DEMO3

Healthy Diets for Healthy Microbiome Demonstrator

13:30 – 13:35	**Introduction to the FNS-Cloud Microbiome Demonstrator** (Maria Traka, QIB, UK)
13:35 – 14:05	**Why is gut microbiome important and how do we research it?** (Falk Hildebrand & Anthony Duncan, QIB, UK)
14:05 – 14:15	**Introduction to Fairspace** (Maria Traka, QIB, UK & Elisa Carillo, The Hyve, NL)
14:15 – 14: 35	**Demonstration of FAIRSPACE via three use cases** (Anthony Duncan, QIB, UK)
14:35 – 15:00	**Hands-on session and discussion** (all)

Login into Fairspace

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Healthy Diets for Healthy Microbiome

Maria Traka

Quadram Institute
Science Health
Food Innovation

Maastricht University
Jožef Stefan Institute
Università degli Studi Firenze
The Hyve
scalefocus
PREMOTEC

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Aim of the Diet & Microbiome DEM03

Healthy Diets for Healthy Microbiome

The aim of the Microbiome Demonstrator is to demonstrate **FNS-Cloud workflows** that bring together ***FNS-data*** generated in diet and microbiome studies, currently residing across multiple fragmented repositories/sources, with ***tools*** **dedicated in FAIRification**, thus facilitating analyses of microbiomes that improves our understanding of the **interaction between diet and microbiome**.

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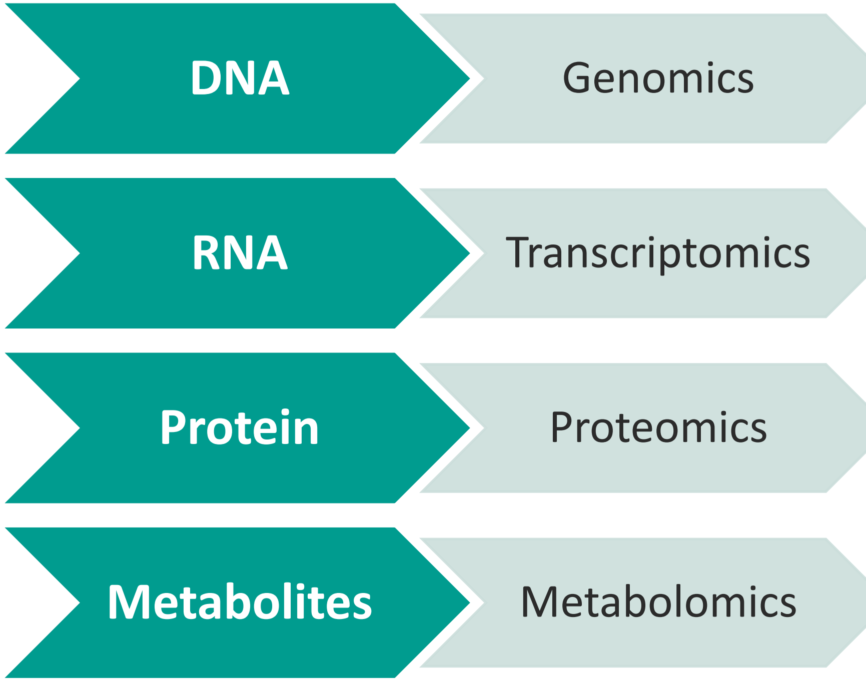
Data types are varied

- **Dietary data**
  - Food diaries/Surveys (raw) – Records of what people ate
  - Nutrition composition (processed) – How much protein is there?
- **Microbiome data**
  - Metagenomics – What bacteria/genes are there?
  - Metatranscriptomics – What genes are being expressed?
  - Metaproteomics – What proteins are present?
  - Metabolomics – What small molecules are present?
- **Health & Lifestyle data**
  - Clinical data – Blood biomarkers
  - Wearable – Continuous blood glucose monitor, Sleep monitor



DNA Genomics

RNA Transcriptomics

Protein Proteomics

Metabolites Metabolomics

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Data storage/Repositories

- **ELIXIR Deposition Databases**
  - European Nucleotide Archive – Raw sequencing reads
  - MGnify – Automated Metagenomics pipeline
  - MetaboLights – Raw & Processed Metabolomics
  - PRIDE Archive – Proteomics
  - BioSamples – Metadata
- **Nutritional Phenotype Database**
  - Study and sample metadata – Study design
  - Metabolomic markers – Blood tests etc
- **Dietary data**
  - Food consumption
  - Nutrient intake data

elixir

JPI
a healthy diet
for a healthy life

EMBL-EBI

ENA
European Nucleotide Archive

MGnify

MetaboLights

BioSamples

PRIDE Archive
PRoteomics IDEntifications Database

Phenotype
database

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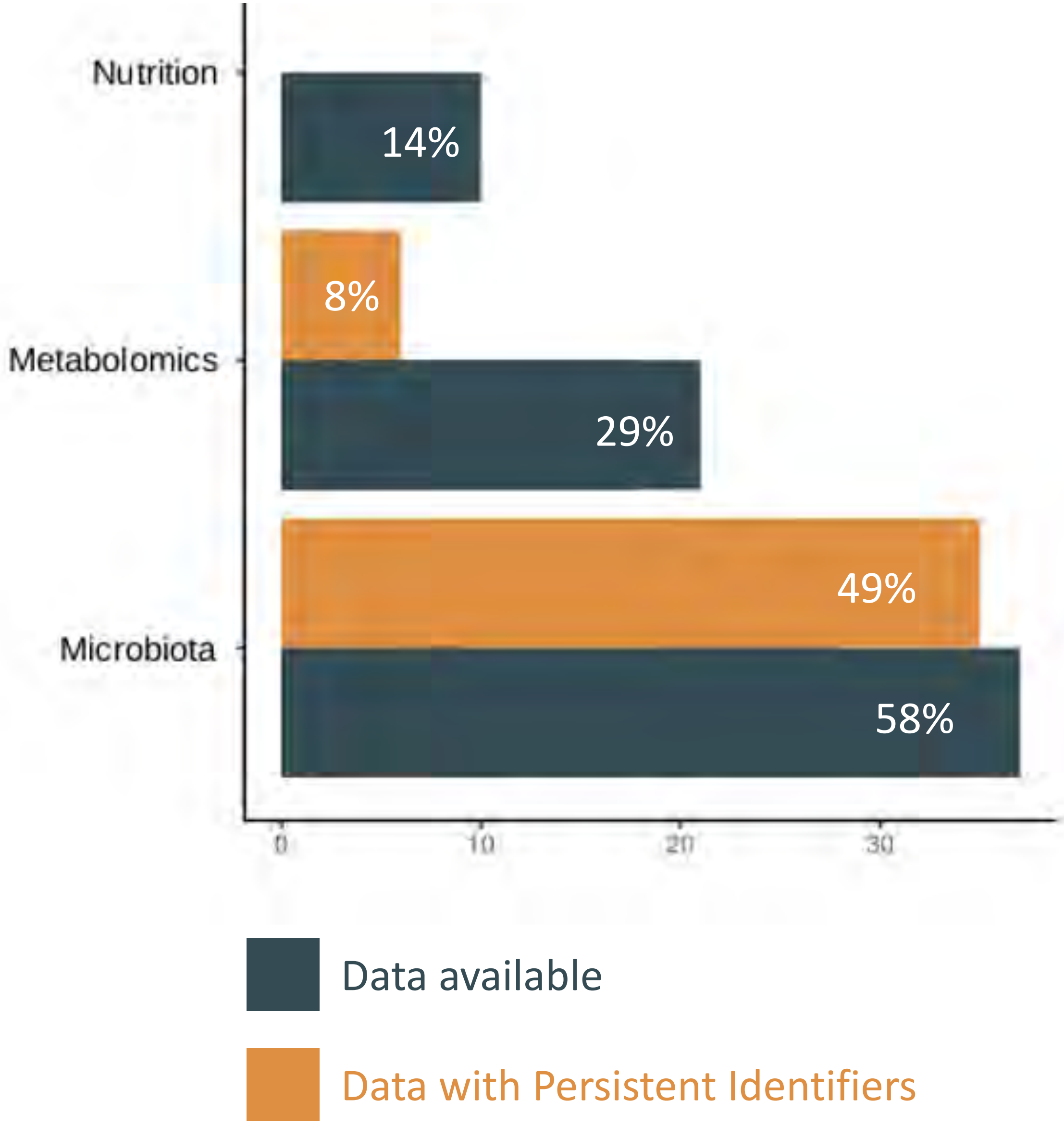

2020-2023

72 papers original-articles reporting metagenomics and metabolomics in a nutrition context

Crucially no way of connecting datasets across different platforms/repositories to facilitate **reuse**

Data not FAIR

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Quadram Institute
Science Health
Food Innovation

DIME Study: Dietary BIoactives and Microbiome DivErsity

Objectives:
- ❖ Does a diverse diet rich in plant bioactive compounds lead to a diverse gut microbiome?

- ❖ Does our microbiome influence our metabolic response to food?

Participants n= 20

High Bioactive Arm
(2 weeks)

Glucosinolates

Polyphenols

Carotenoids

Total Fibre 30g

Low Bioactive Arm
(2 weeks)

Total Fibre 30g

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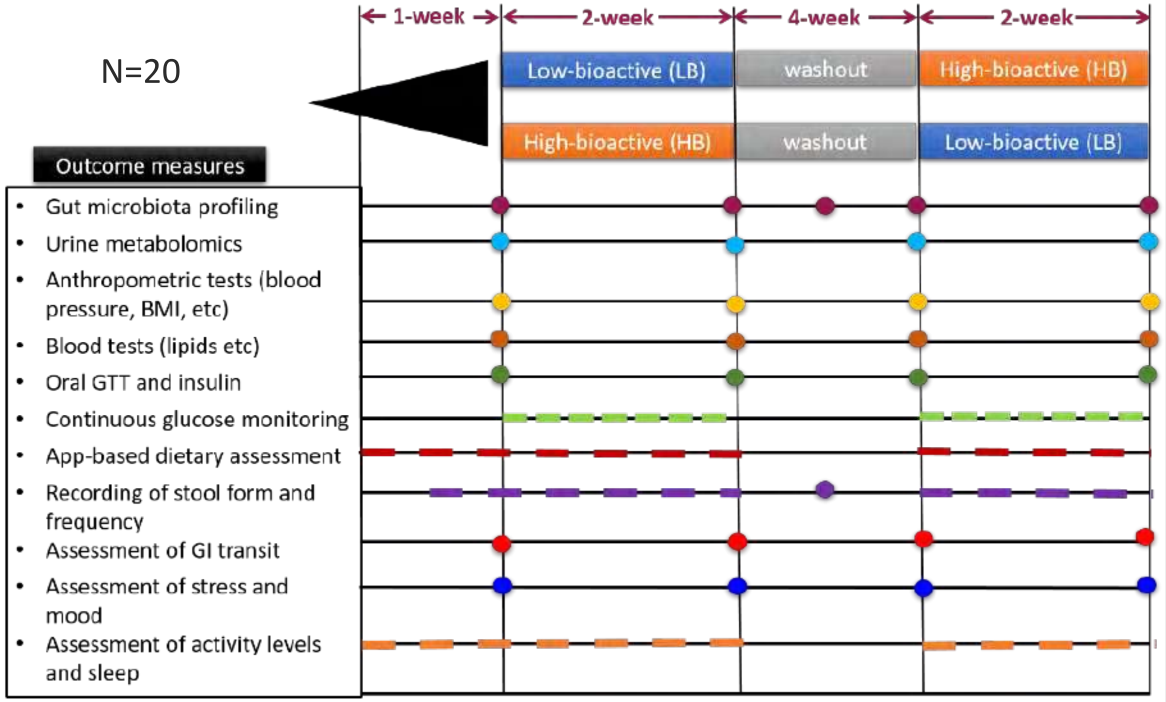
eBASIS Bioactive Substances in Food

Quadram Institute
Science Health Food Innovation

DIME Study: Dietary BIoactives and Microbiome DivErsity



N=20

1-week | 2-week | 4-week | 2-week

Low-bioactive (LB) | washout | High-bioactive (HB)

High-bioactive (HB) | washout | Low-bioactive (LB)

Outcome measures

- Gut microbiota profiling
- Urine metabolomics
- Anthropometric tests (blood pressure, BMI, etc)
- Blood tests (lipids etc)
- Oral GTT and insulin
- Continuous glucose monitoring
- App-based dietary assessment
- Recording of stool form and frequency
- Assessment of GI transit
- Assessment of stress and mood
- Assessment of activity levels and sleep

DATA

Food & Nutrition

Diet app tool development –wearables integration (sleep, CGM)

NUTRITICS LIBRE

Biomarker & Anthropometric

Weight, age, inflammation, HbA1c, TGs, hip/waist), etc.

Microbiome

Bacterial community composition and function

- Whole genome sequencing
- Metagenomics and metabolomics

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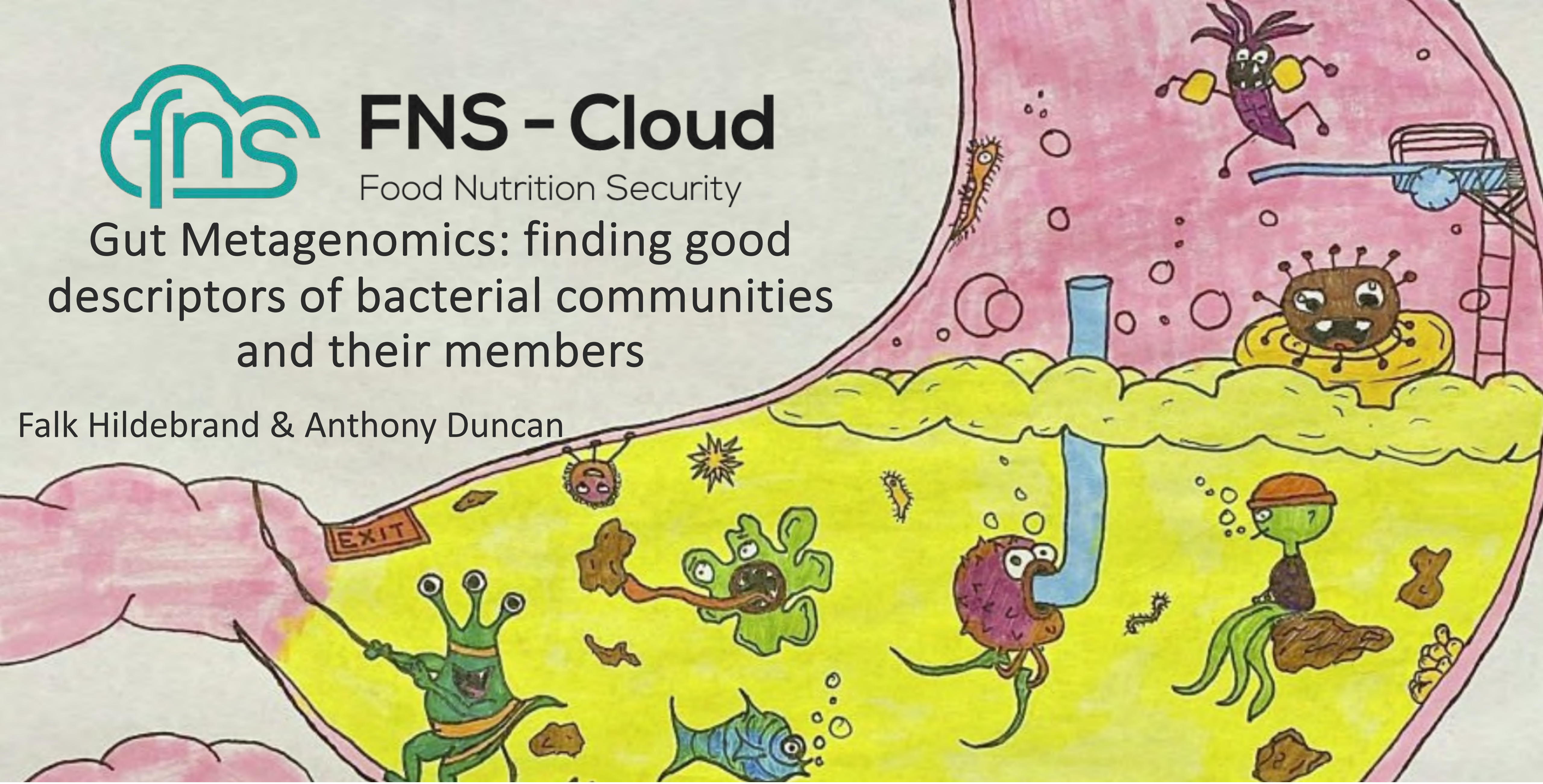
Gut Metagenomics: finding good descriptors of bacterial communities and their members

Falk Hildebrand & Anthony Duncan



(Sabri Conde-Yassin / The McGill Tribune)

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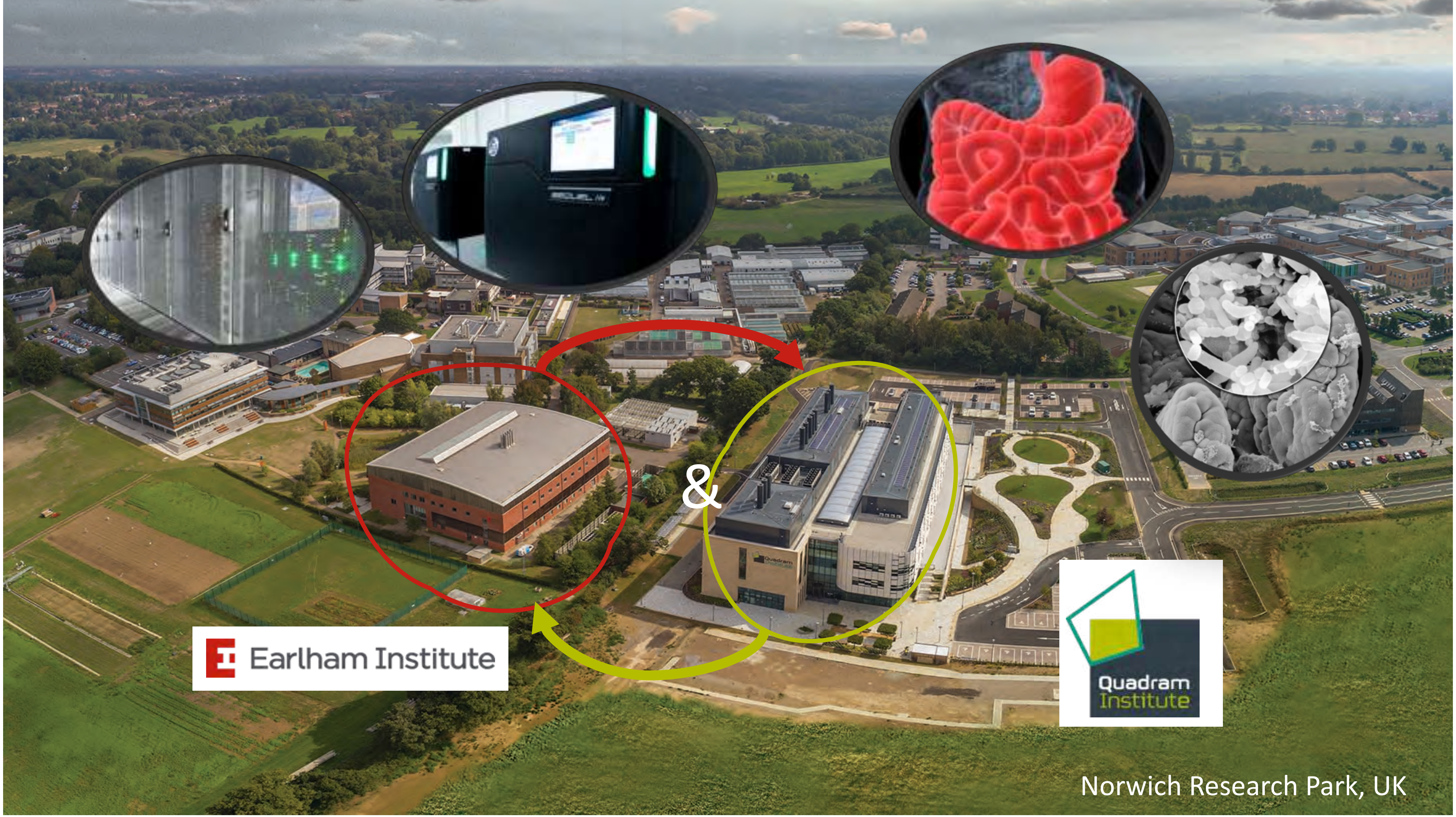

Norwich Research Park, UK

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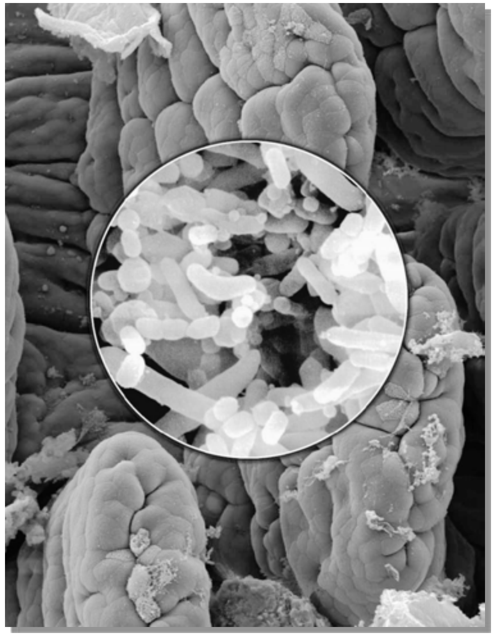
Importance of the human microbiota for us



- Catabolism of fibers
- Anabolism of Vitamins & Cofactors
- Maturation & Modulation of Immune System
- First line defense pathogens
- **… many more found by now** (like dietary Bioactive conversion)

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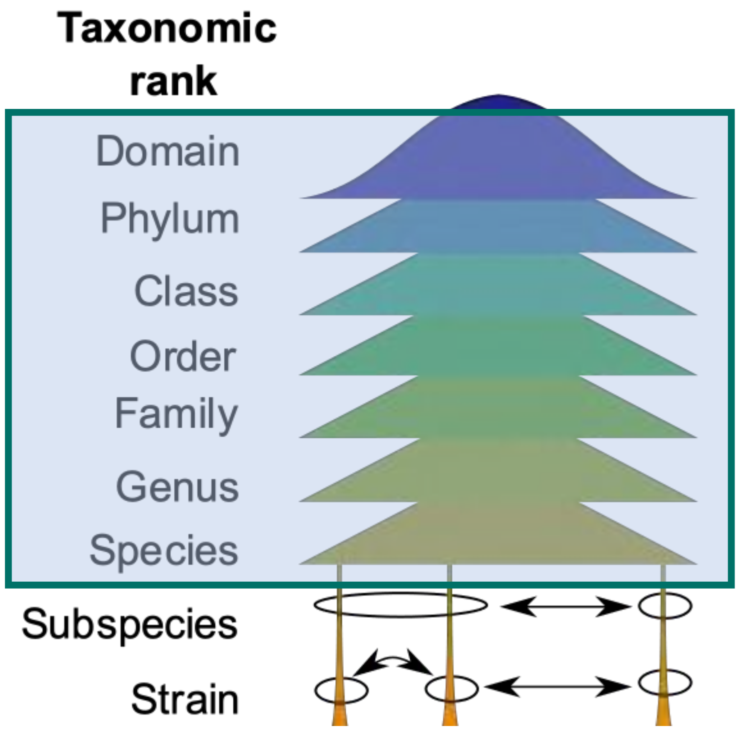
Taxonomy is integral to understand microbiomes

- Community composition is the mix of different taxa

- Most often analysis is at species or genus level



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Hildebrand, F. *mSystems* e0088121 (2021).

Analyzing Genus/Species level microbiomes

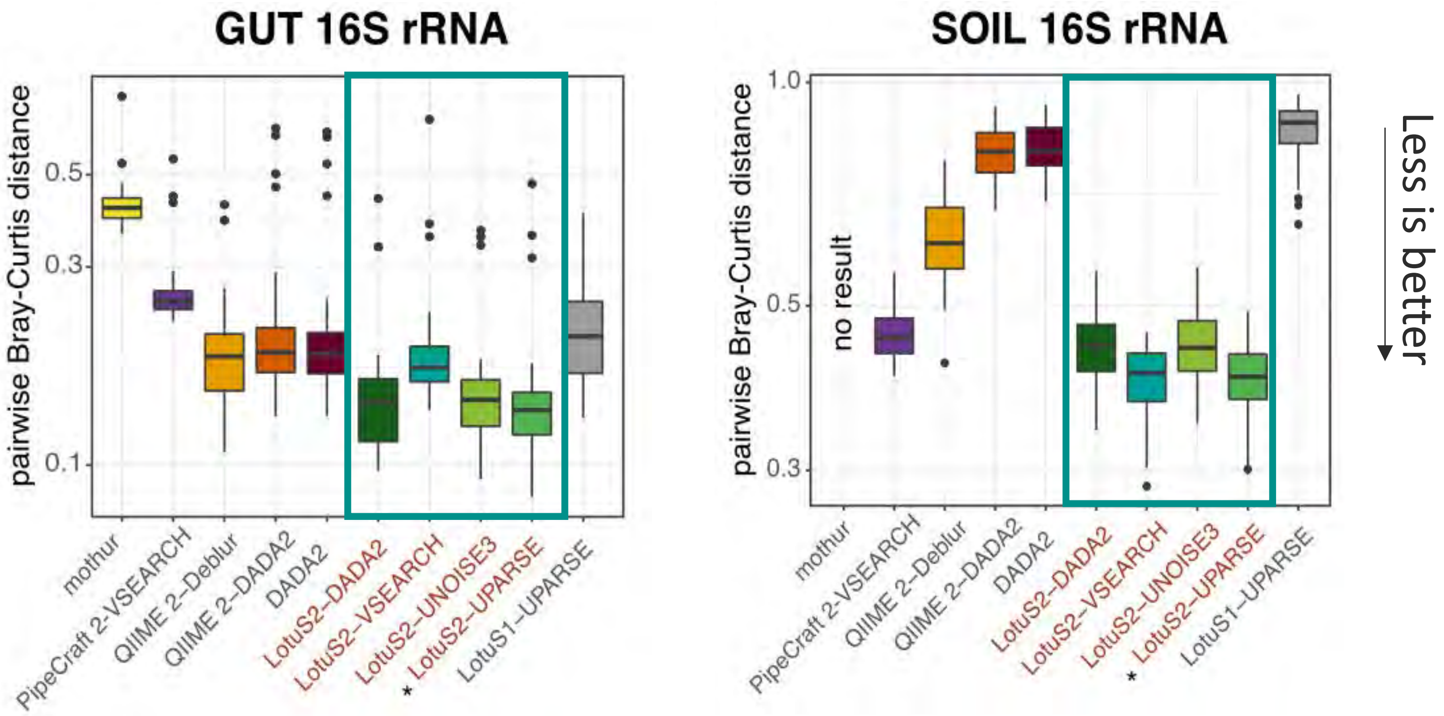
Ezgi Özkurt

Joachim Fritscher

Amplicon sequencing (16S) is sufficient

- Straightforward & standardized analysis
- Fast & efficient bioinformatic solutions available
  - LotuS2 developed in our lab

Reproducibility among gut/soil replicates



Özkurt, E. **Fritscher** J, Soranzo N, **Ng** D, Davey R, Bahram M, **Hildebrand** F. LotuS2: An ultrafast and highly accurate tool for amplicon sequencing analysis. *Microbiome* (2022)

http://lotus2.earlham.ac.uk/

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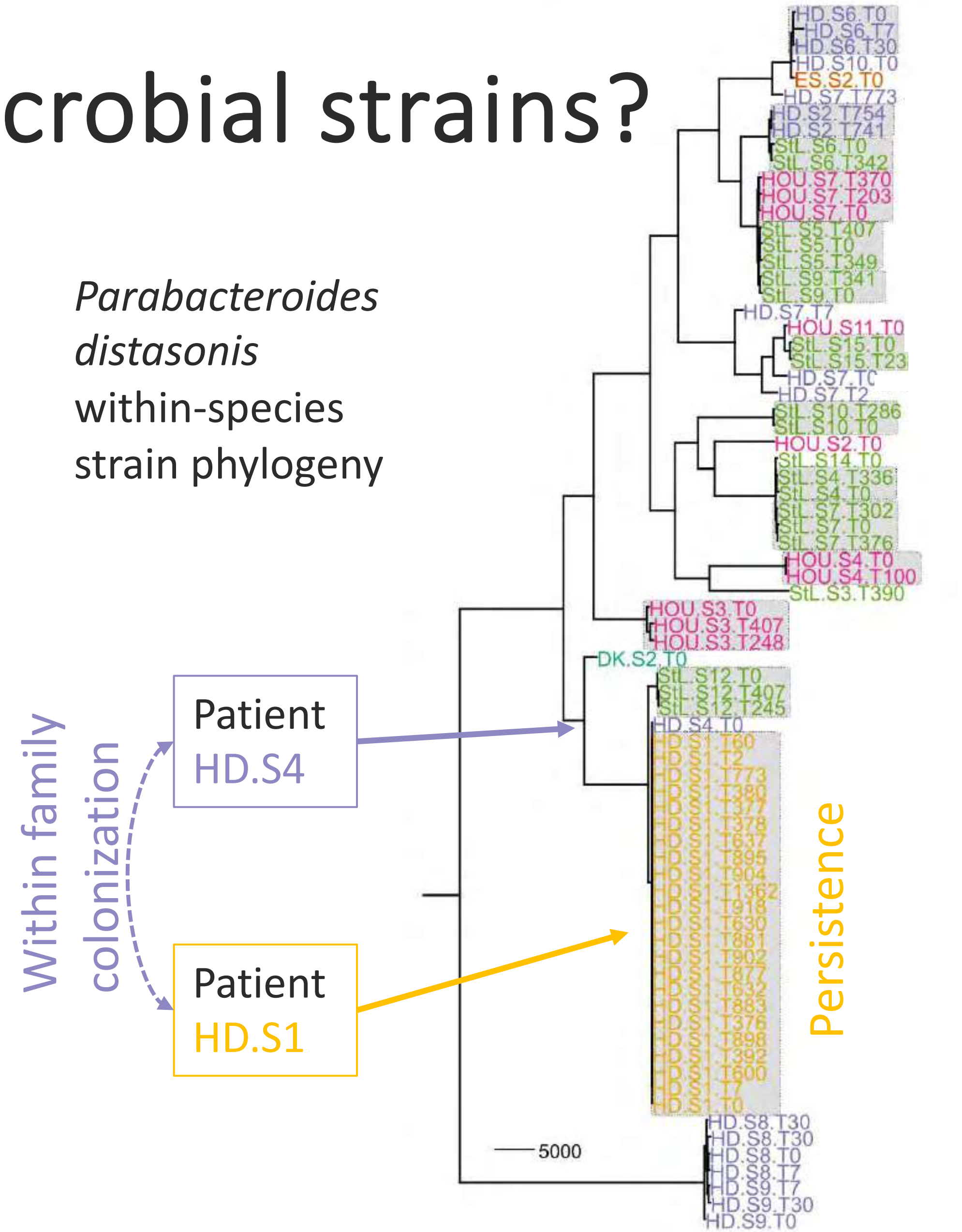
Why should we care about microbial strains?

Same species
Different strains…

- → Clinical outcome varies
- → Medication, fibre metabolism
- → Immune modulation
- → Prebiotic effectiveness

Strain resolved metagenomics is the pathway to personalized medicine

Parabacteroides distasonis
within-species
strain phylogeny



Hildebrand F et al, Antibiotics-induced monodominance of a novel gut bacterial order. *Gut* 2019

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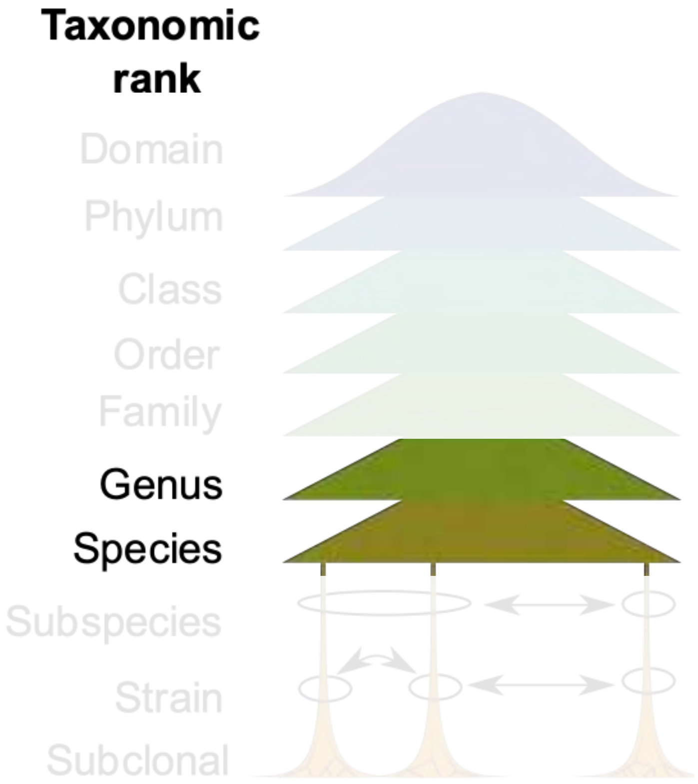
Strains in the human gut

Tracking microbial strains in health & disease



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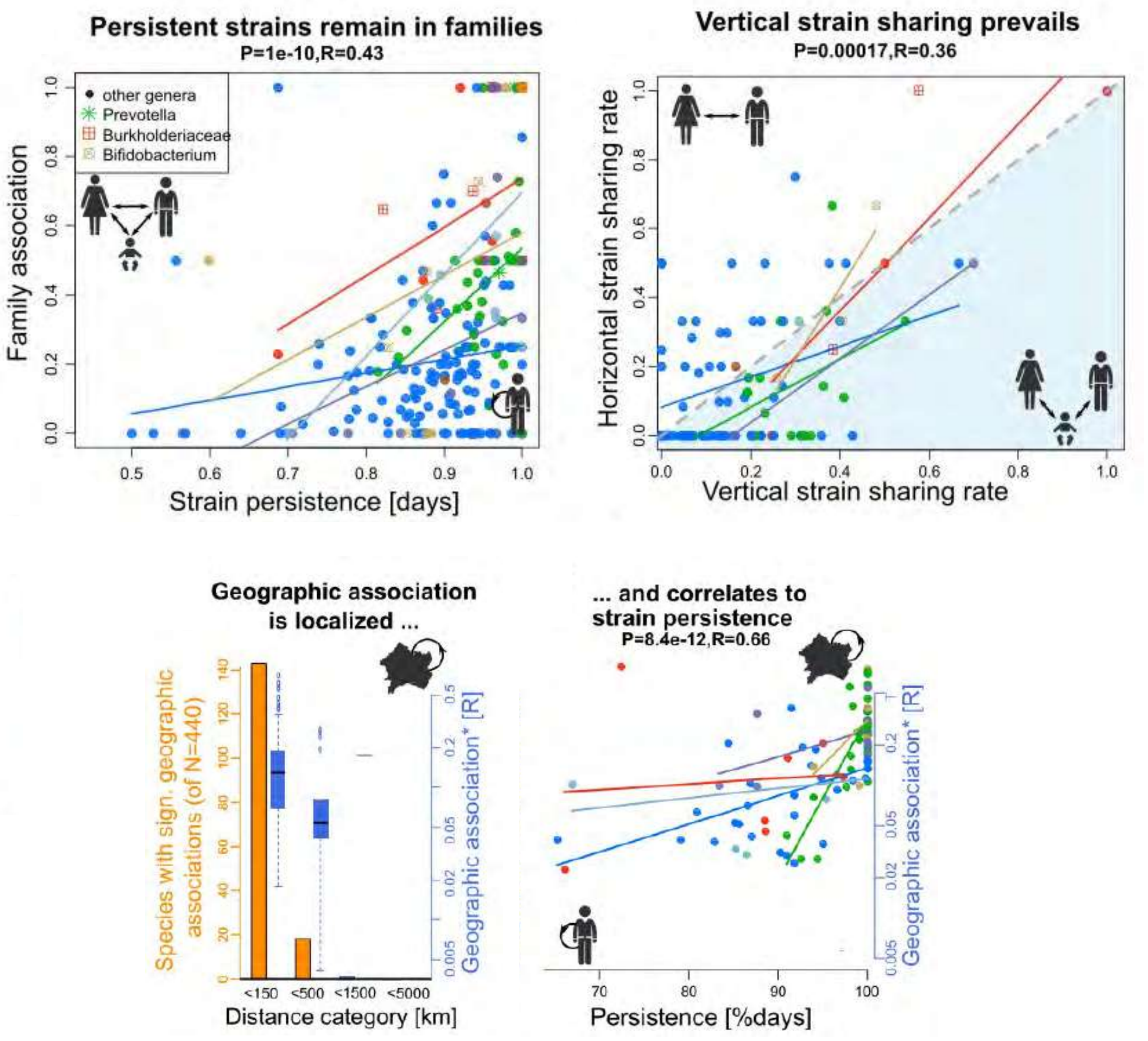
Persistence of the human gut microbiome



- >5,000 metagenomes: children, adults, families, timeseries
- Gut bacteria are persistent (>95% of observed days)
- Gut bacteria that are persistent, stay within families
- Colonization happens at all ages (but usually more parent->child)
- Some gut bacteria “stick around” in a geolocation
  - localized “outbreaks” of successful strains

Hildebrand, Gossman, Frioux, Ozkurt, et al., *(2021) Cell Host & Microbe*

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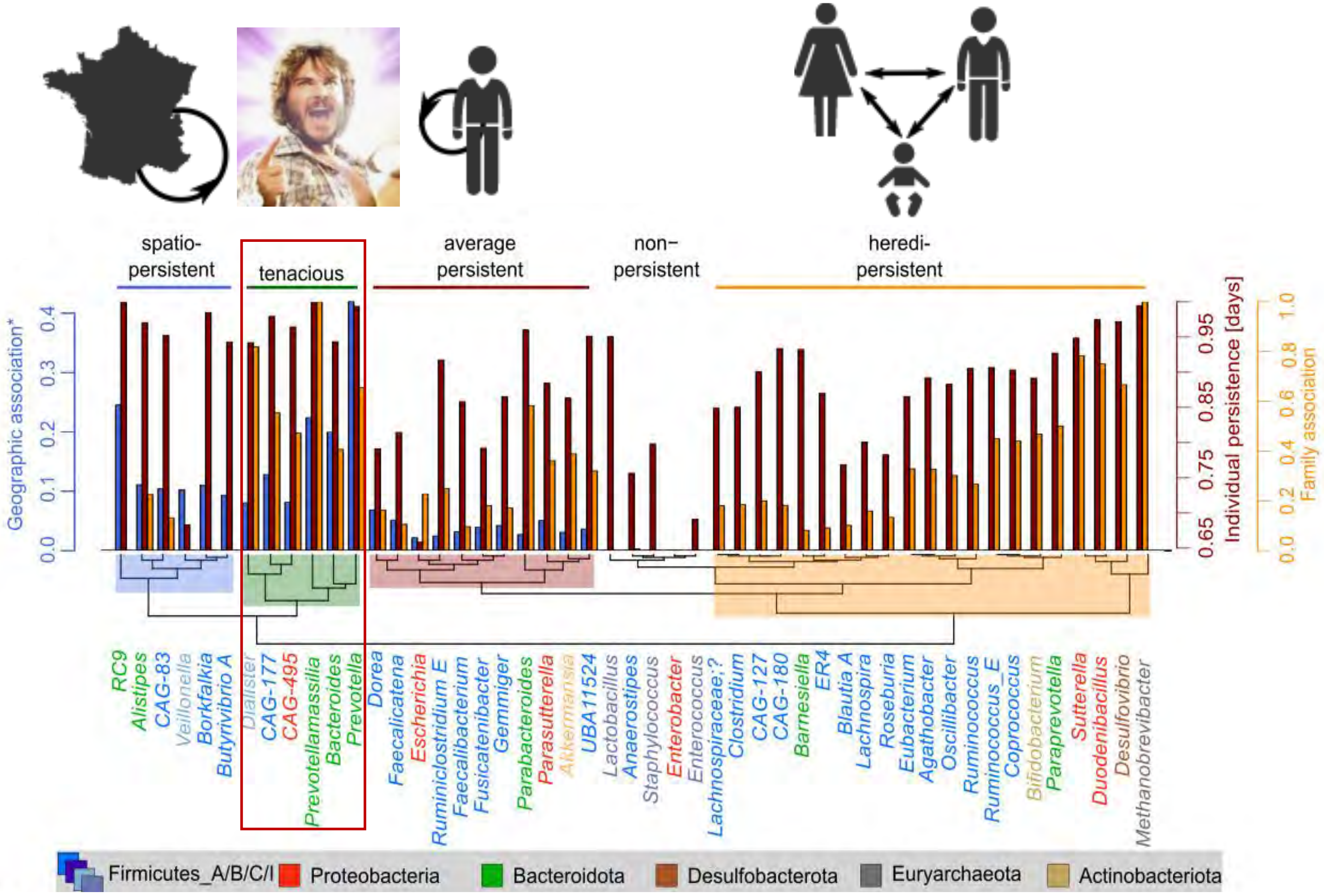
Dispersal strategies of gut bacteria

- Gut bacterial colonization strategies
  - Host associated
  - Family associated
  - Geographically anchored
  - Excel in all (tenacious)



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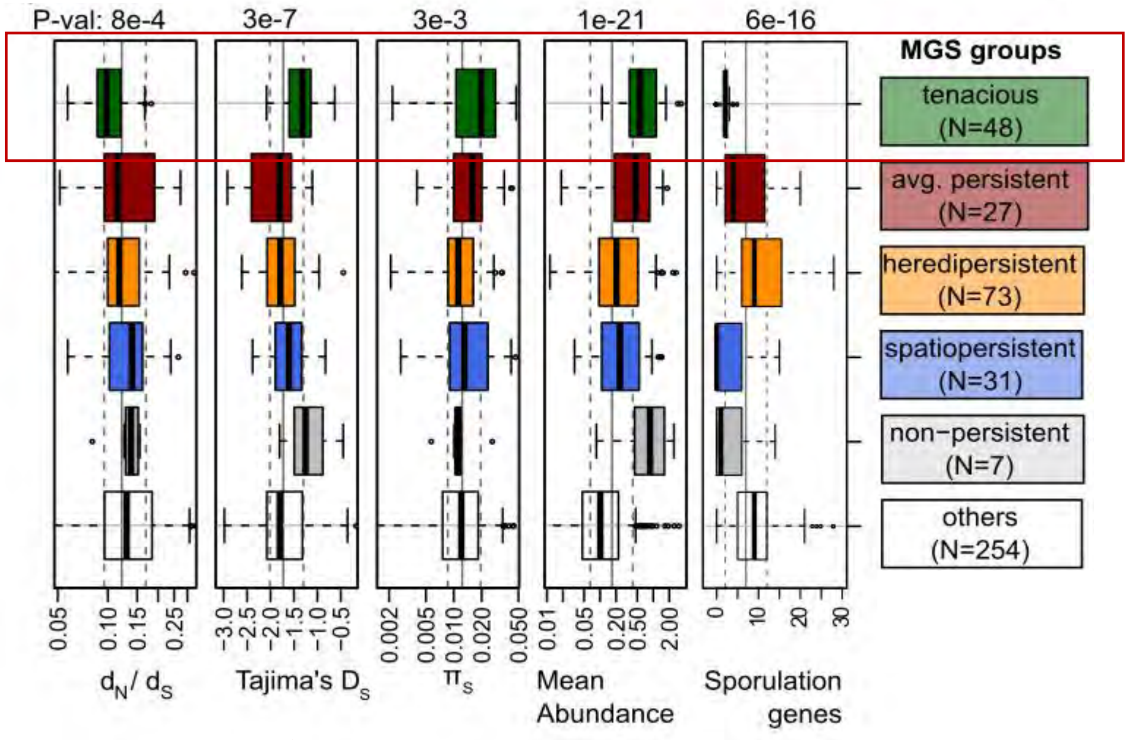
Dispersal influences evolution of gut bacteria

- Gut bacterial colonization strategies
  - **excel in all (tenacious)**
- Tenacious gut bacteria are highly adapted to the human host
- … and most affected by antibiotics



AA optimization

Genetic bottlenecks

Eff. population size

Actual population size

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Hildebrand, Gossman, **Frioux**, **Ozkurt**, et al., *(2021) Cell Host & Microbe*

Summary

The personalized microbiome

Using high-resolution metagenomics we can:

- Reconstruct colonization patterns of microbes in individuals, families, geographic regions
- Quantify evolution of microbes & their genes

- Understand dispersal strategies pathway to manipulating microbiome (pre-, probiotics)
- Identify microbial strains with medical relevance (IBD)

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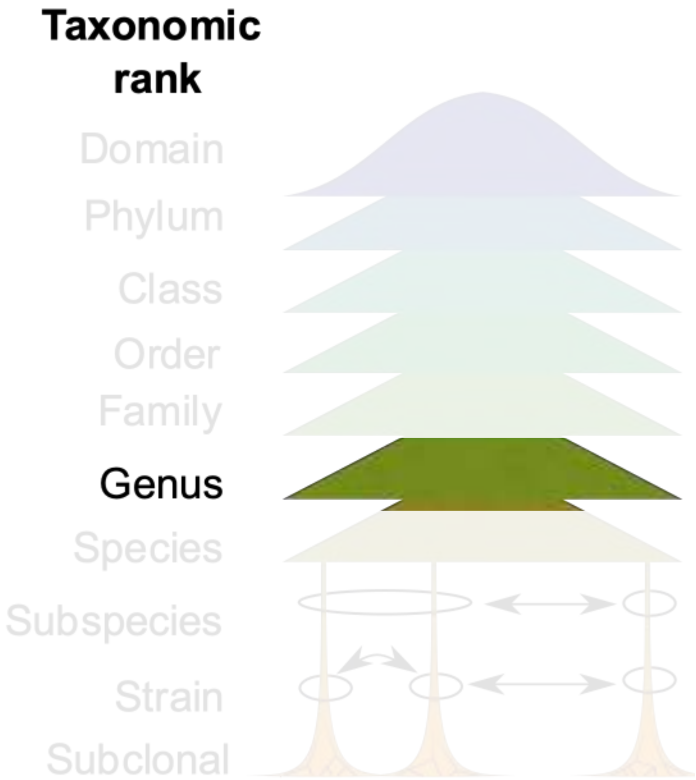
A universal gut microbiome signature

Sometimes genus level works better..



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Humans are great at simplifying stuff

“Forest”

“Grassland”

“Forest”

“Grassland”

Use of **ecosystem types**

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Graphicriver.net; Wikipedia.co.uk

Ecotypes harbor specific species

Forest animals

Grassland animals

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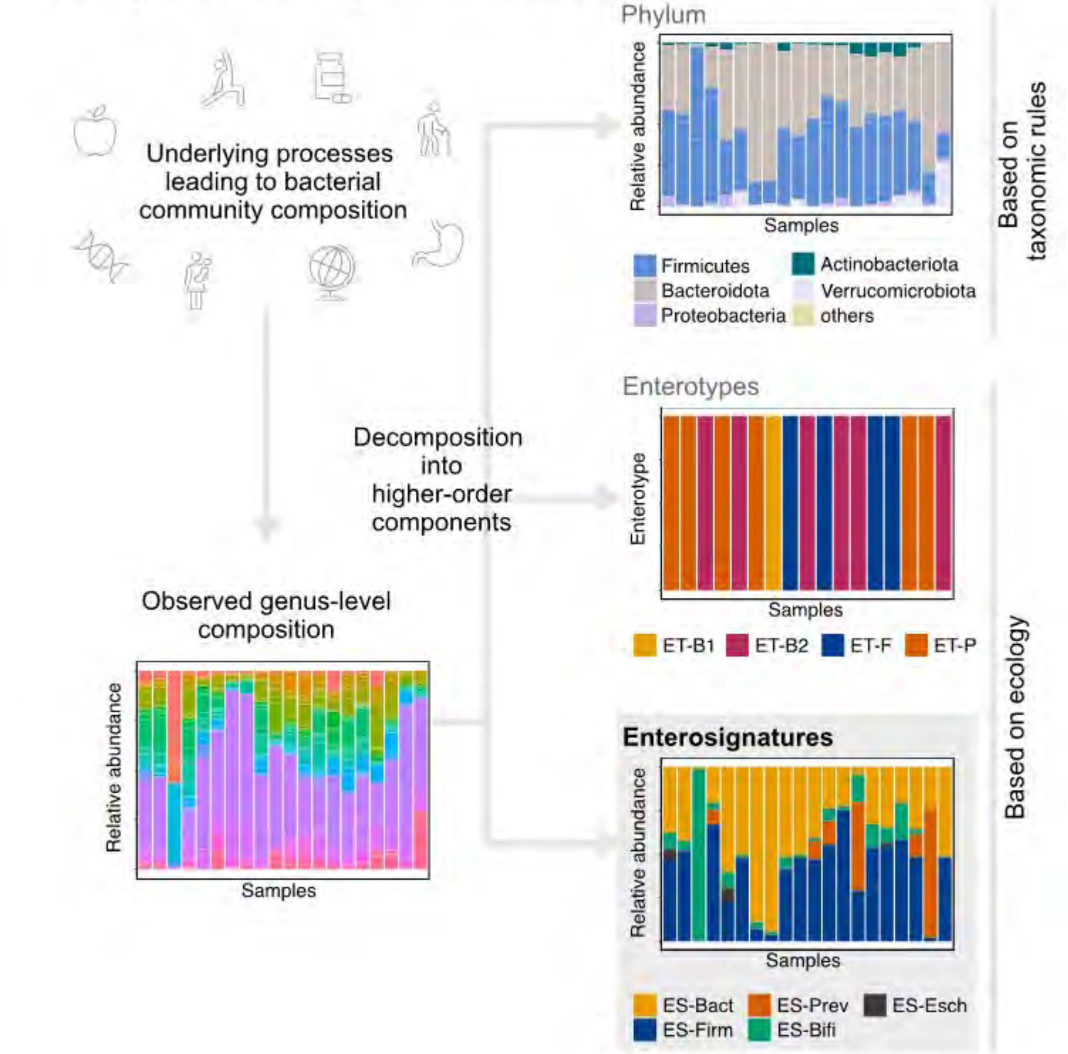
Graphicriver.net; Wikipedia.co.uk

Enterosignatures (ES) recapture ecosystem gradients

Clemence Frioux

Rebecca Ansorge



Frioux C, **Ansorge** R, **Özkurt** E, Nedjad CG, **Fritscher** F, Quince C, Waszak SM, **Hildebrand** F (2023) **Enterosignatures define common bacterial guilds in the human gut microbiome**

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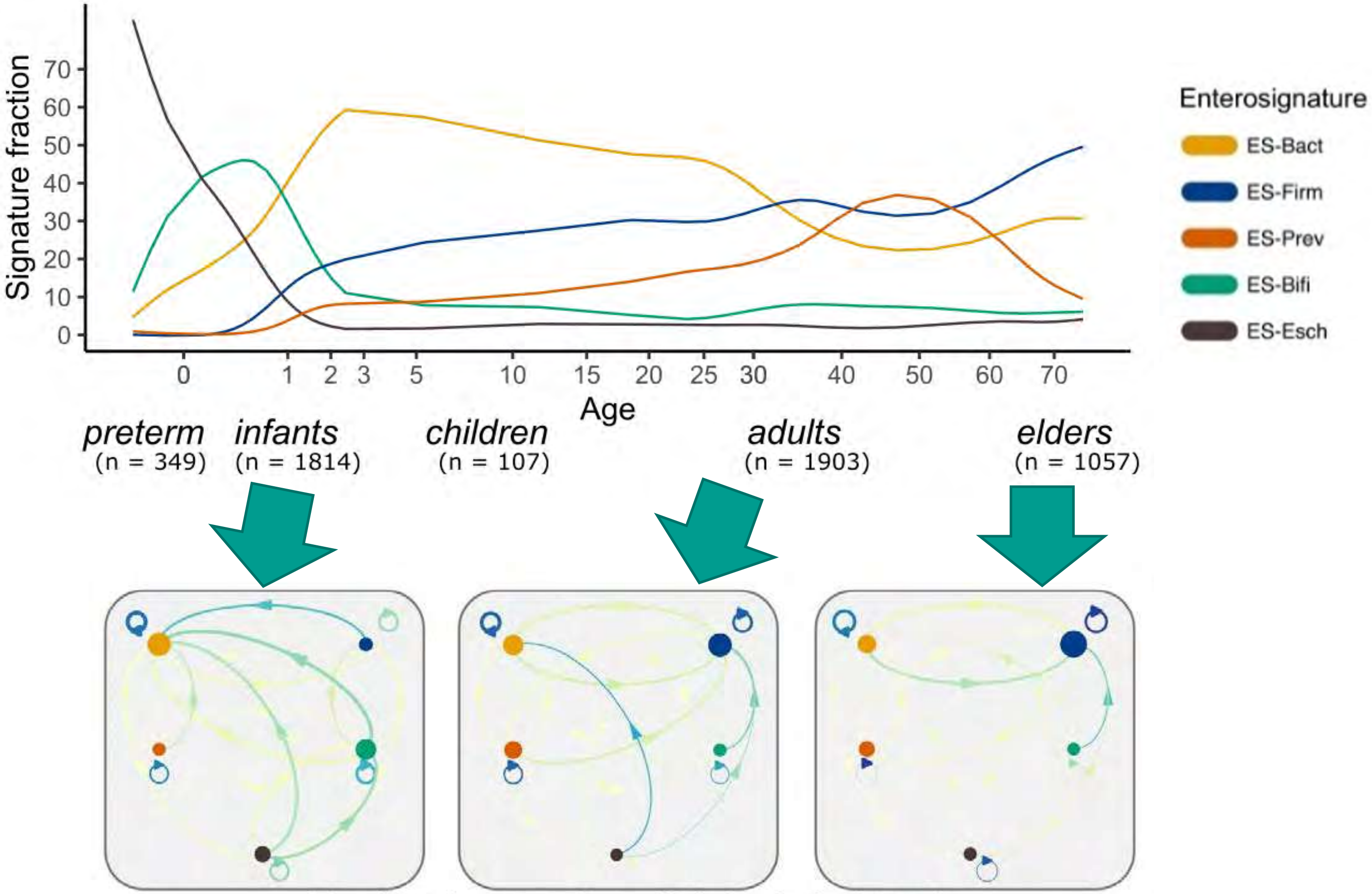
Enterosignatures change with host age

- Different ES prevalent at different host ages
- Difference between “adult” and “infant” ES
- Possible ecosystem successions:
  - ES-Esch/ES-Bif → ES-Bact → ES-Firm → ES-Prev
- ES-Bact remains central



Transitions between primary ES in longitudinal samples

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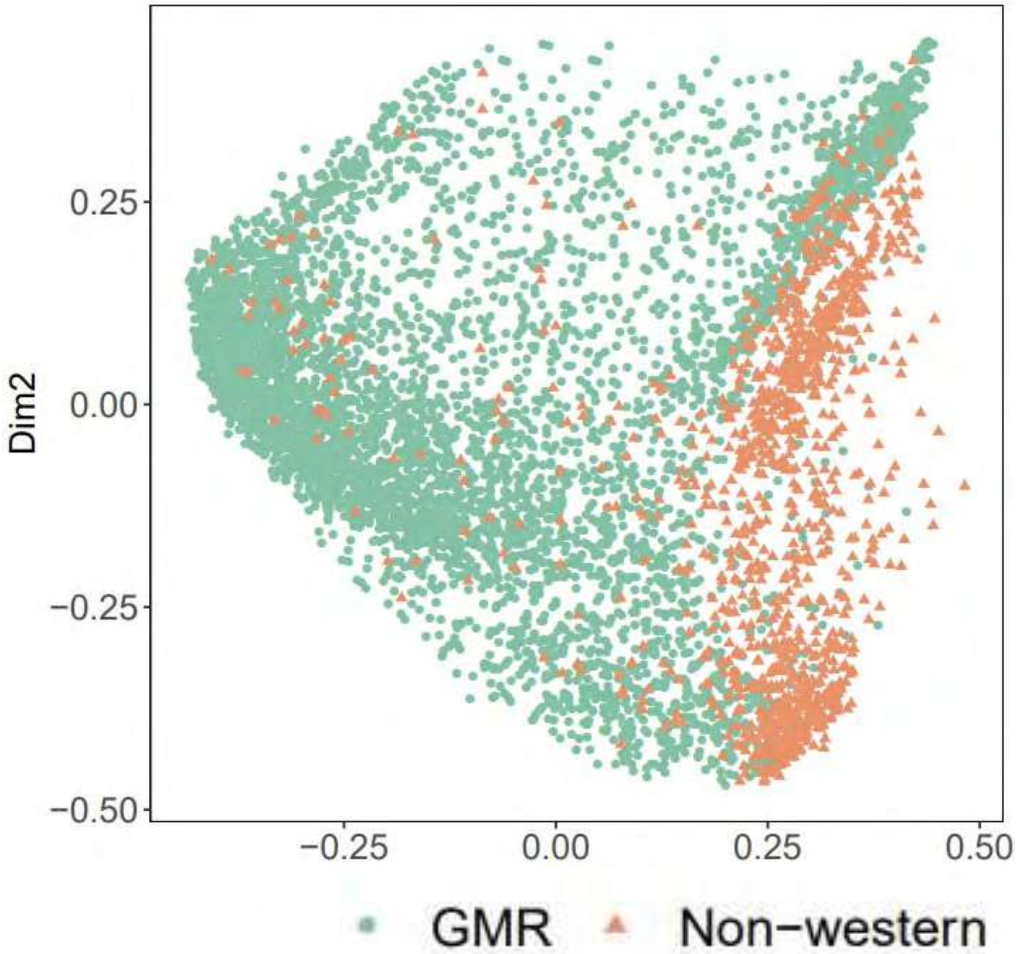
Enterosignatures are universally applicable

- 5 ES derived from Western (GMR) cohort
- Application to non-western cohort



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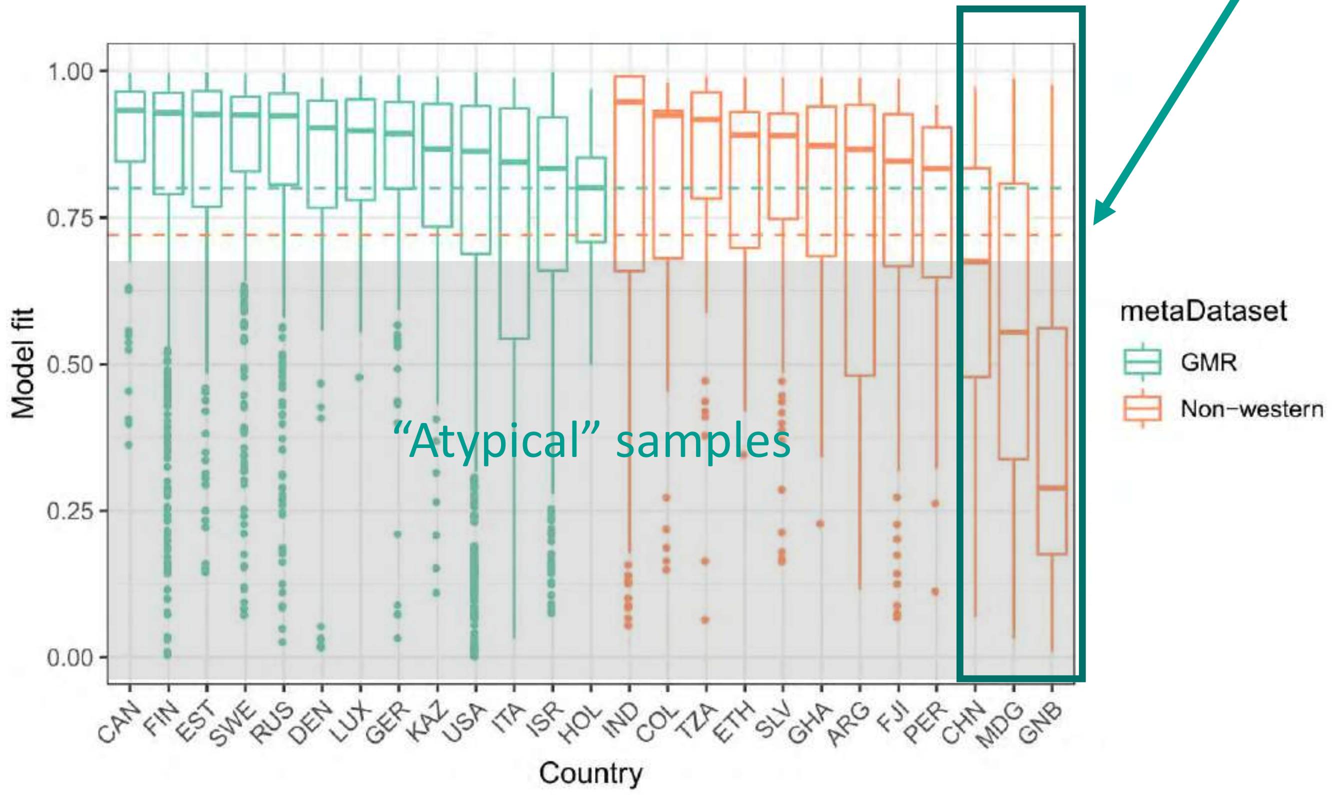
Enterosignatures are universally applicable

- 5 ES derived from Western cohort
- Application to non-western cohort shows good fit
- Cohorts with bad fit :
    - faeces collected in ethanol
    - Helminth infections



"Atypical" samples

Ethanol stool preservation

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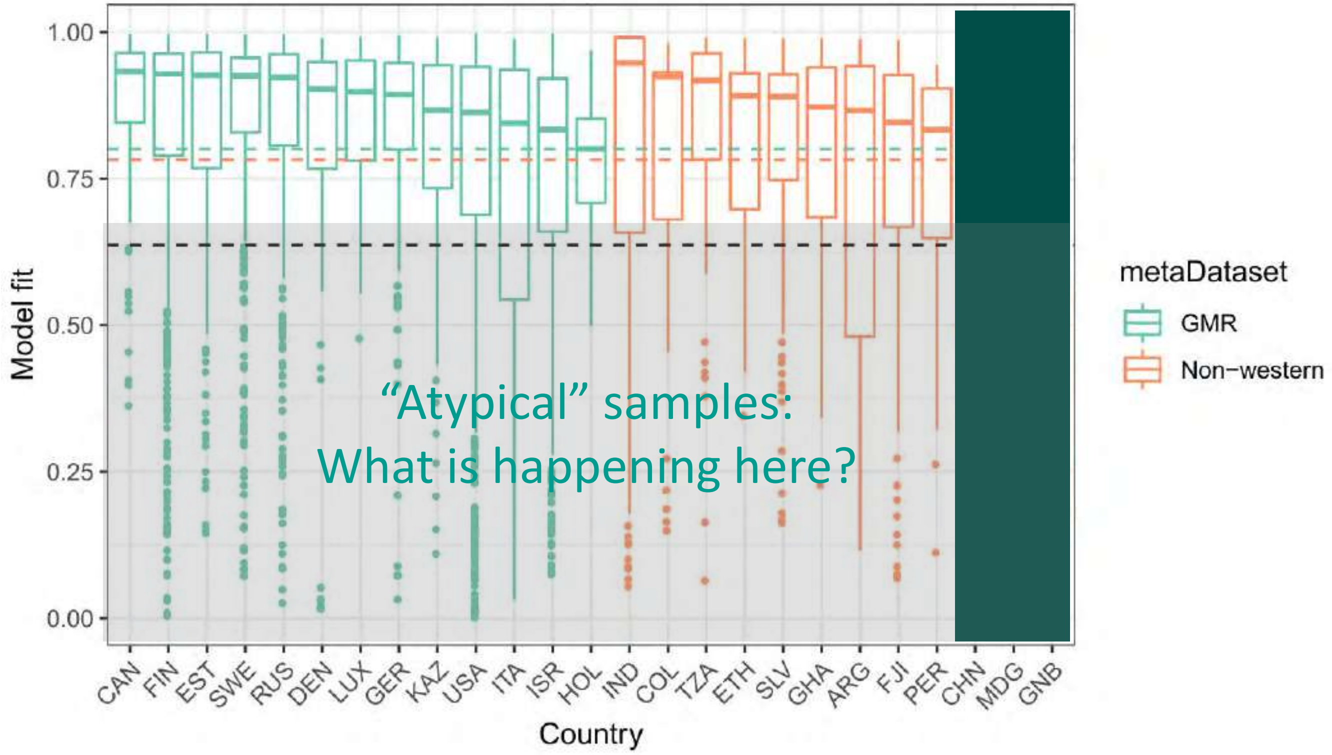
Enterosignatures are universally applicable

- 5 ES derived from Western cohort
- Application to non-western cohort shows good fit
- Cohorts with bad fit :
    - faeces collected in ethanol
    - Helminth infections
- Samples with bad fit ??



"Atypical" samples:
What is happening here?

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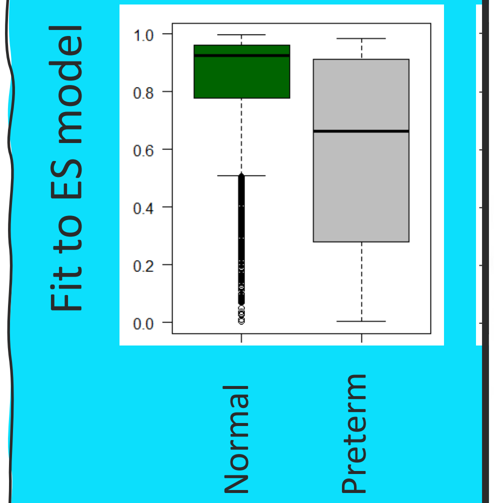
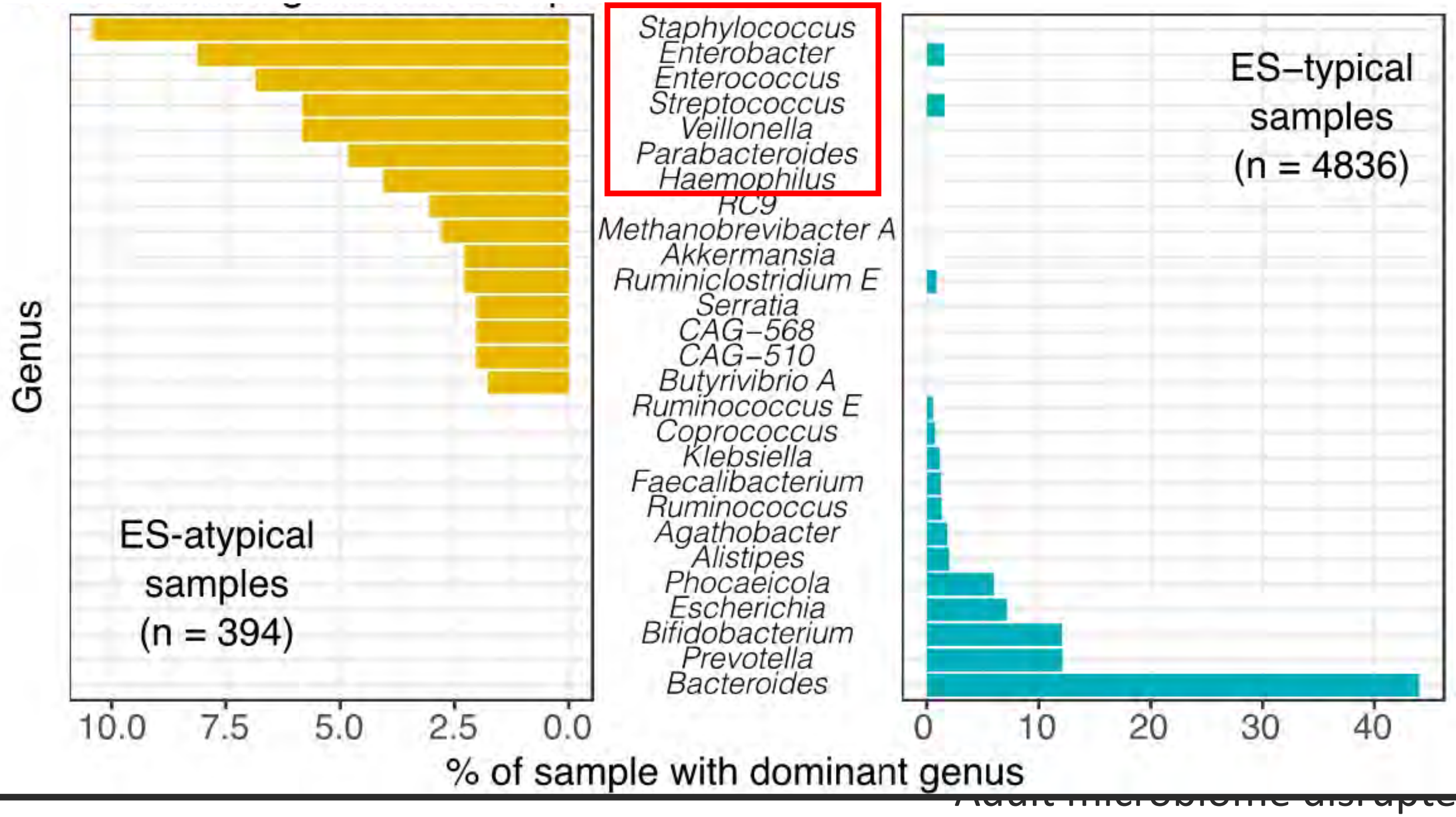
Deviations from enterosignatures describes anormal host states

Preterm birth



Baby microbiome is ne

Potentially pathogenic bacteria dominate atypical samples



ost antibiotic
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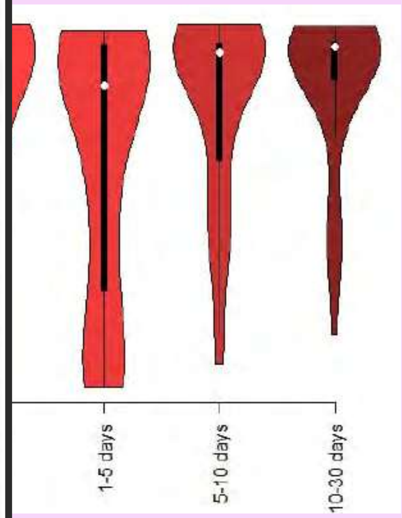

Adult microbiome disrupted by antibiotics

Frioux C, Ansorge R, Özkurt E, Nedjad CG, Fritscher F, Quince C, Waszak SM, Hildebrand F (2023) **Enterosignatures define common bacterial guilds in the human gut microbiome**

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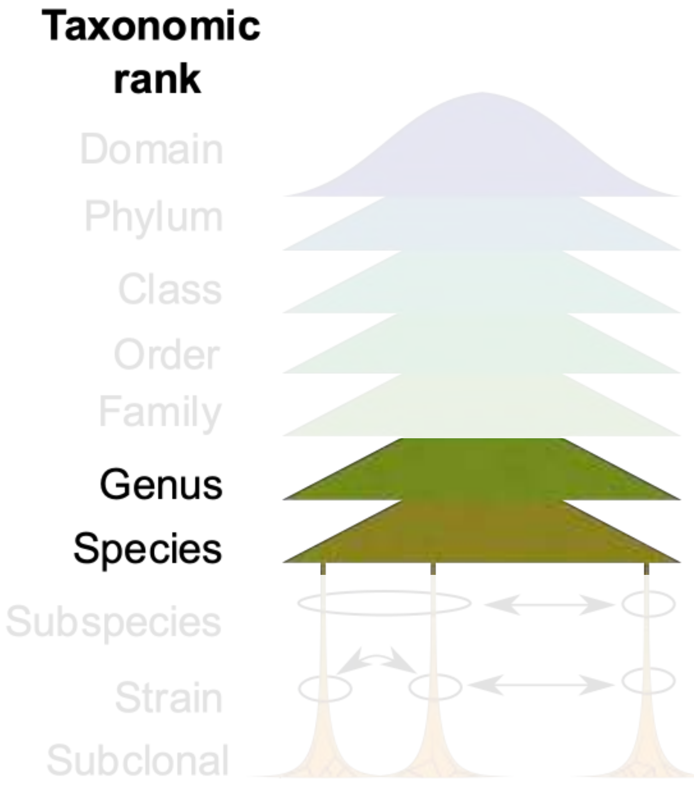

DIME study

Diet intervention on a healthy, young cohort

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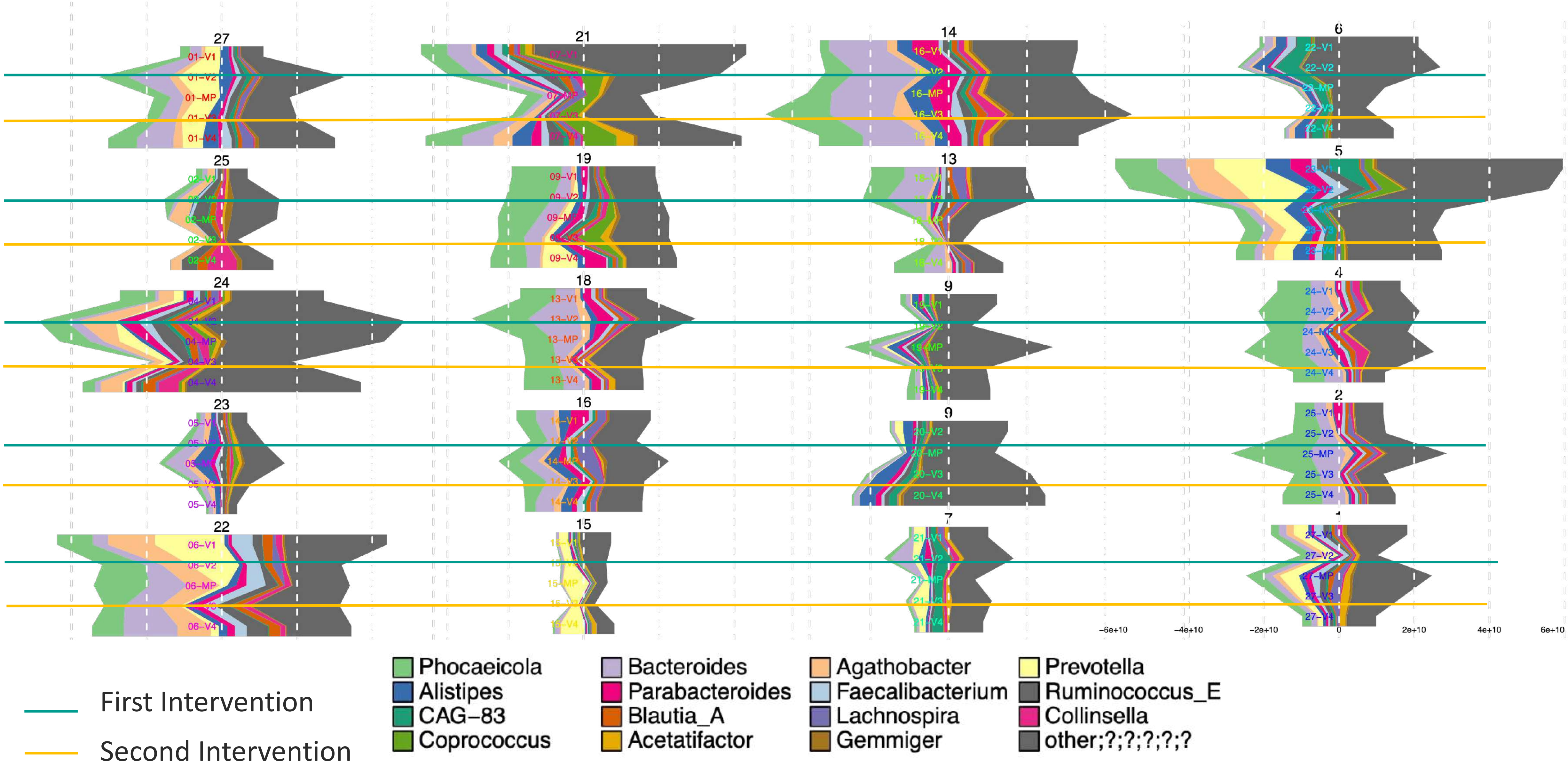
Abundance per Participant (genus)



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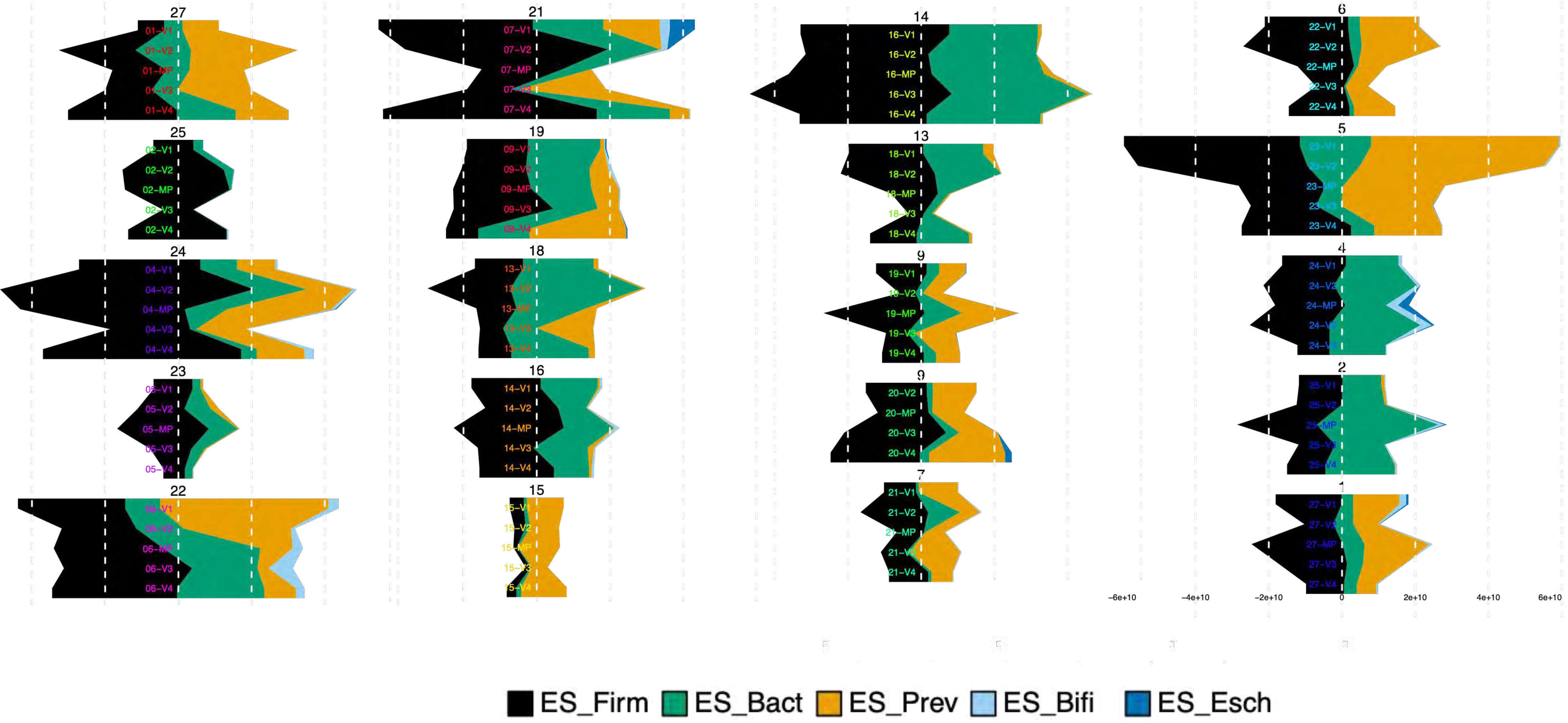
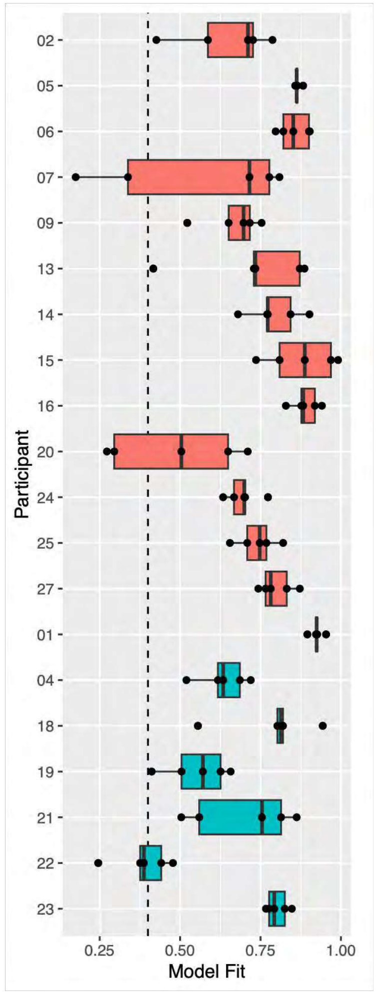
Abundance per Participant (Enterosignatures)



Model Fit



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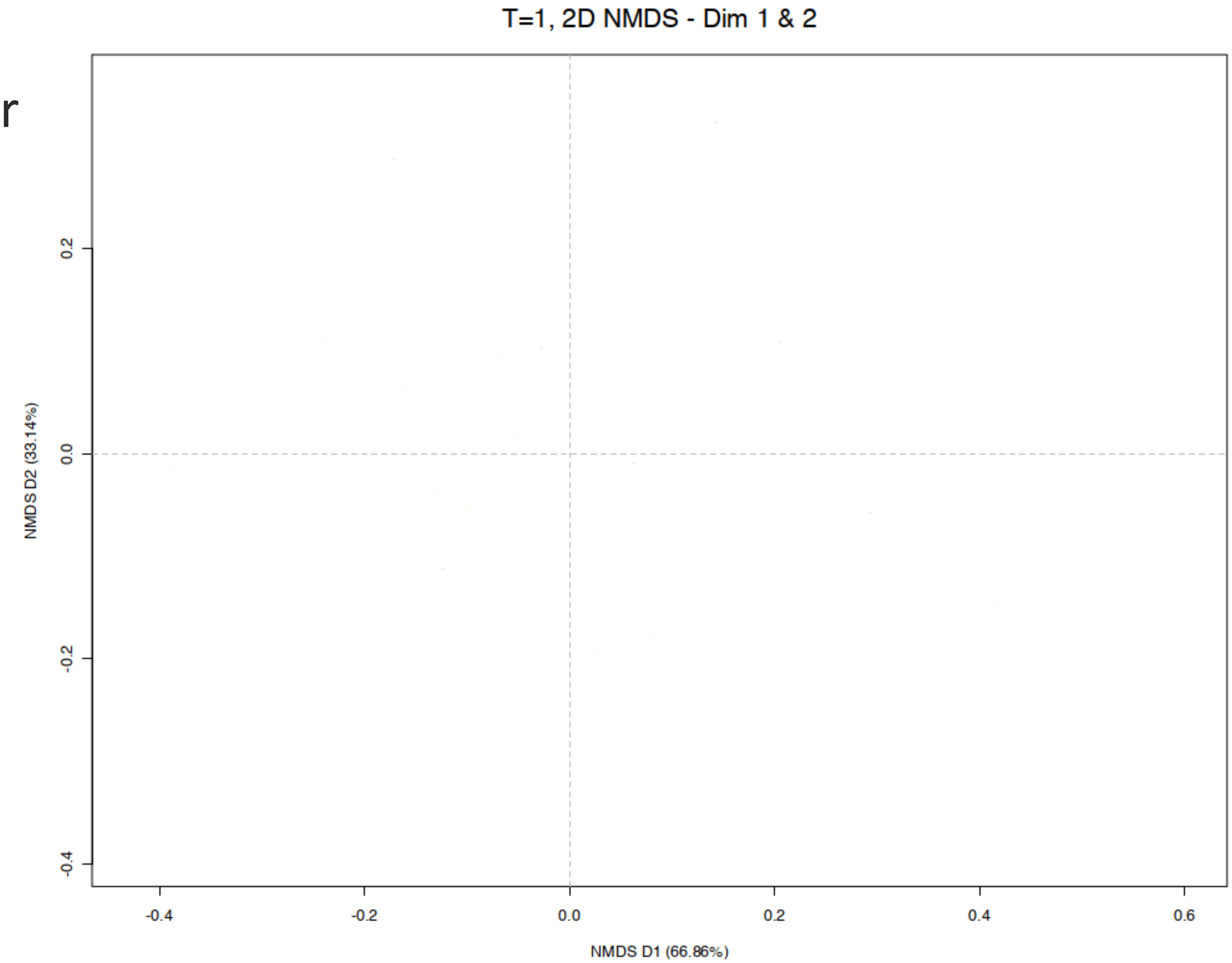
Beta Diversity per participant

Low Bioactive First

HighBioactive First



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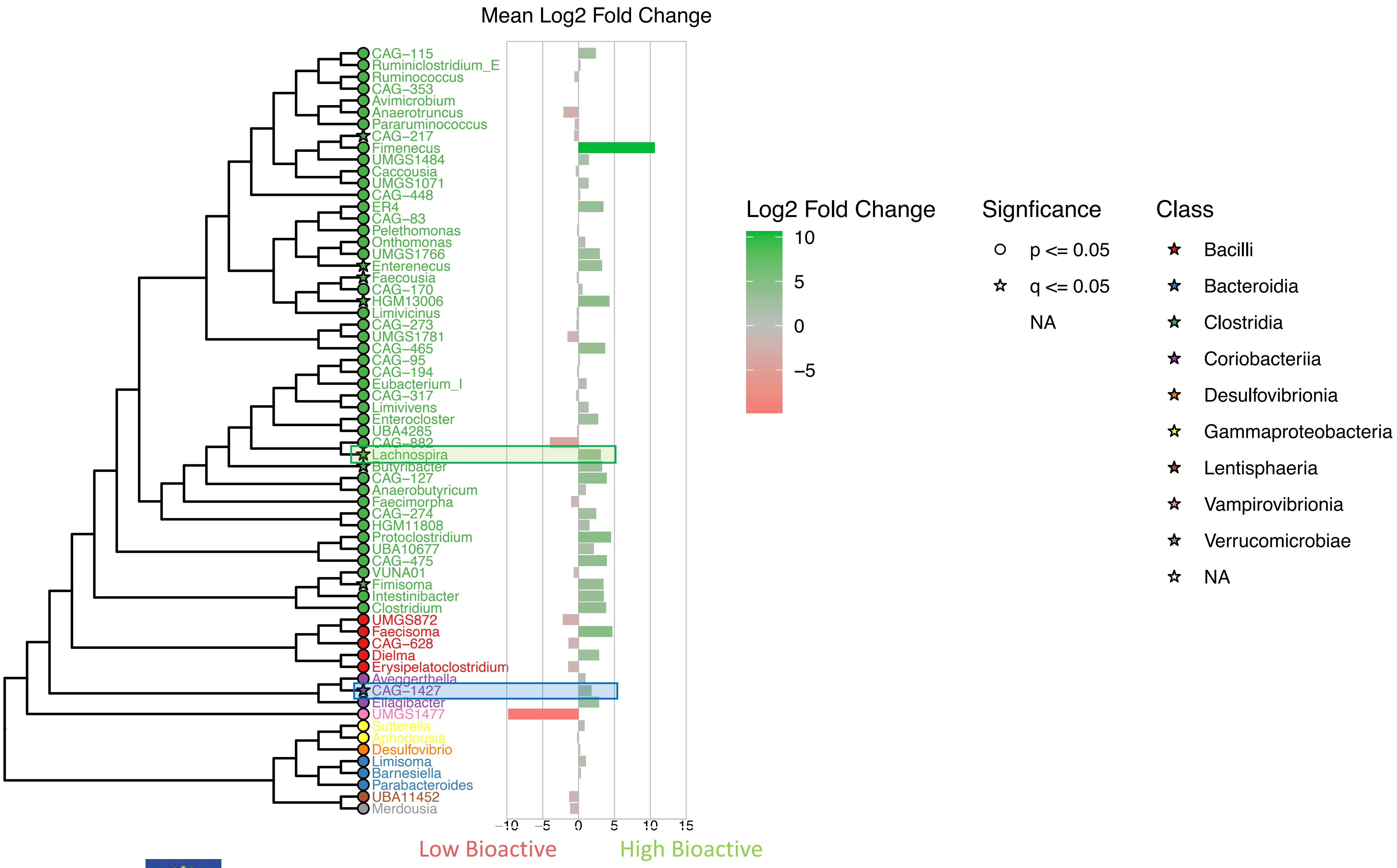

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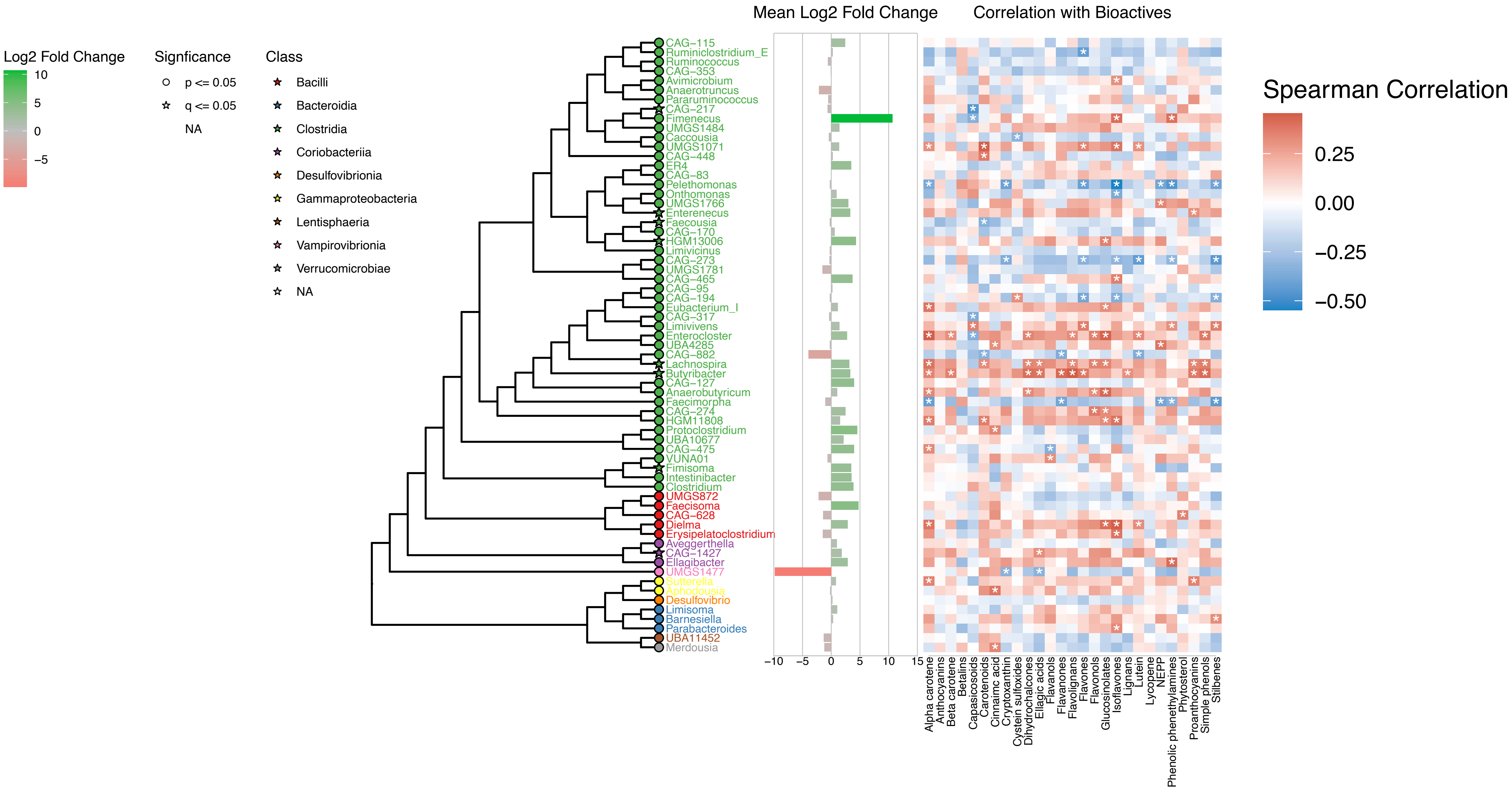

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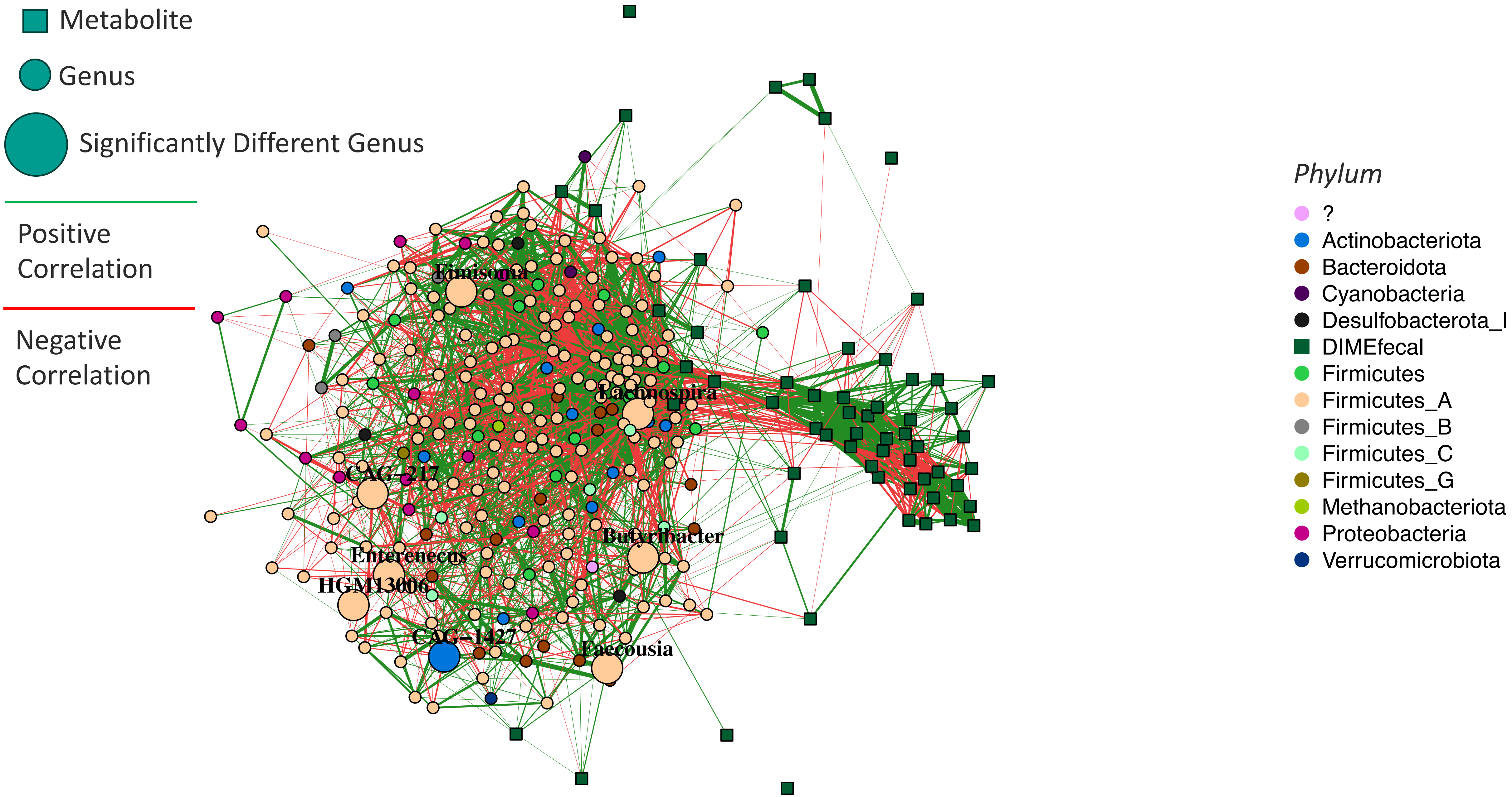

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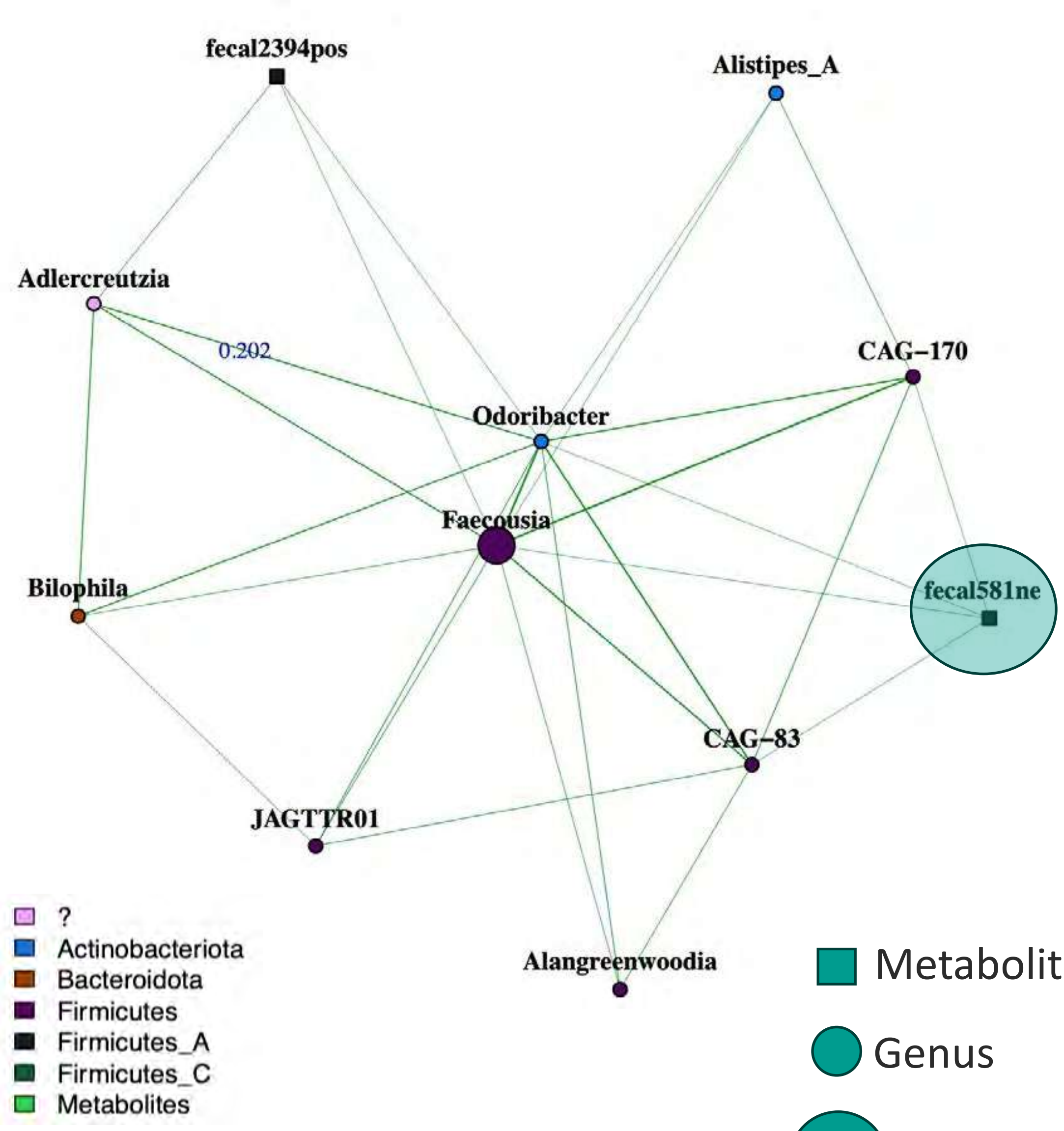

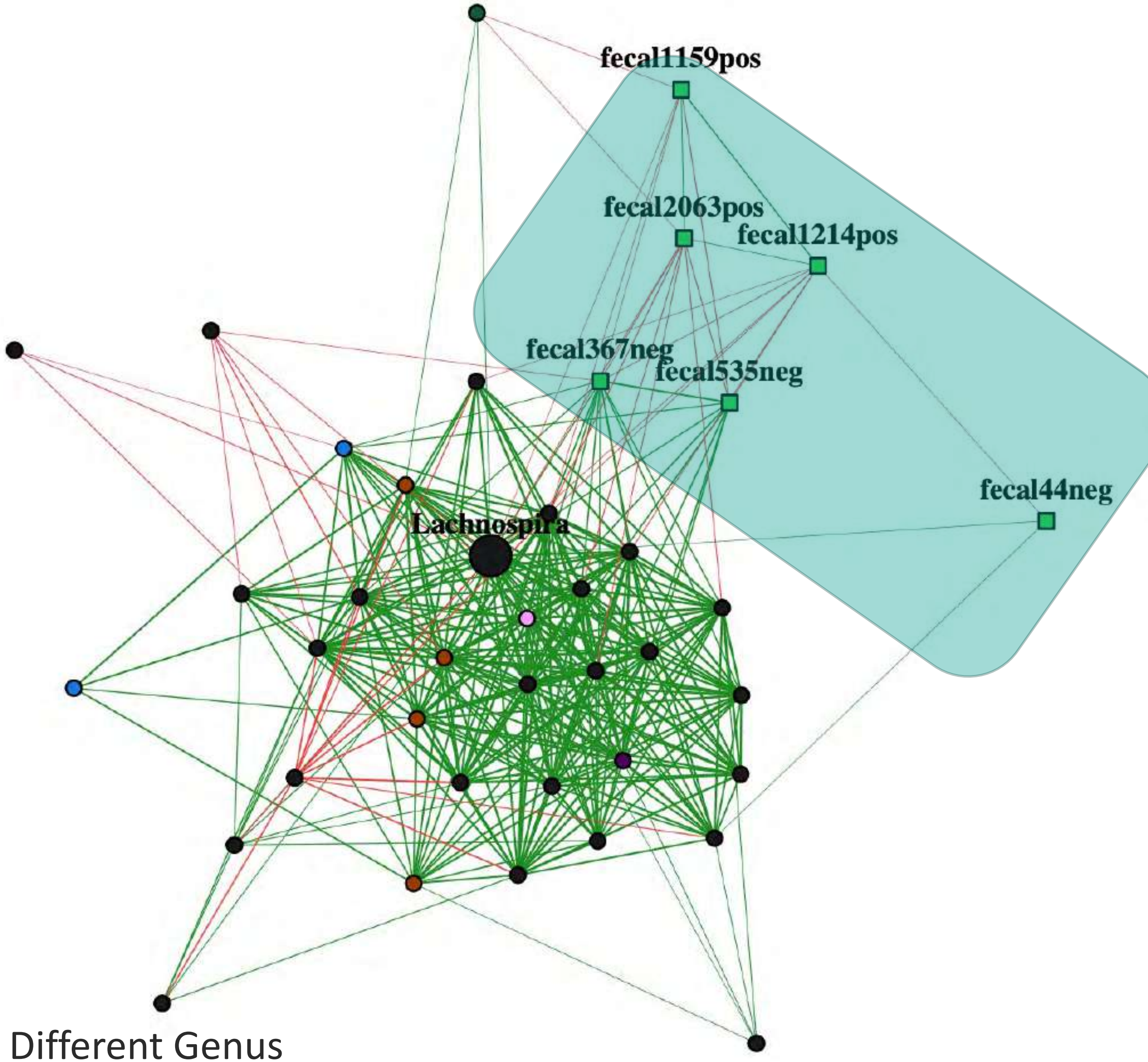

- 🟩 Metabolite
- ● Genus
- ⬤ Significantly Different Genus

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Summary

Enterosignatures:

- capture a lot ecosystem information, while relatively simple model
- Concept of "normally" expected used to describe healthy microbiomes
    - Average is best

DIME study:

- Some taxa do appear to respond to a diet high in bioactives (e.g. CAG-1427)
- Types of dietary fibre may influence some of the other changes in composition
- Potential to identify some microbe-metabolite relationships with further development of network approach

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Thank you

Clemence Frioux, Rebecca Ansorge, Ezgi Özkurt
(alumna, INRIA France)

Anthony Duncan, Joachim Fritscher, Klara Cerk, Ece Silan, David Schneider

Peer Bork, Jeroen Raes, Chris Quince
(EMBL, Uni Leuven, Earlham Institute)

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European Research Council
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UKRI Biotechnology and Biological Sciences Research Council

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Fairspace

Click me

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FNS - Cloud
Food Nutrition Security

Fairspace for Microbiome Demo3

BY

Elisa CirIllo, Team Lead The Hyve

The Hyve

Fairspace

An open source **research data management platform** that adheres to FAIR principles.

It offers a **collaborative environment** to manage any type of research data and serves additionally as a metadata repository.


Fairspace Key Features

Fully Customizable Metadata Model

Metadata Search & Browse Interface

Easy Annotations

Configurable Components

Integrated Analysis Environment

Secure File Storage

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Configurable components

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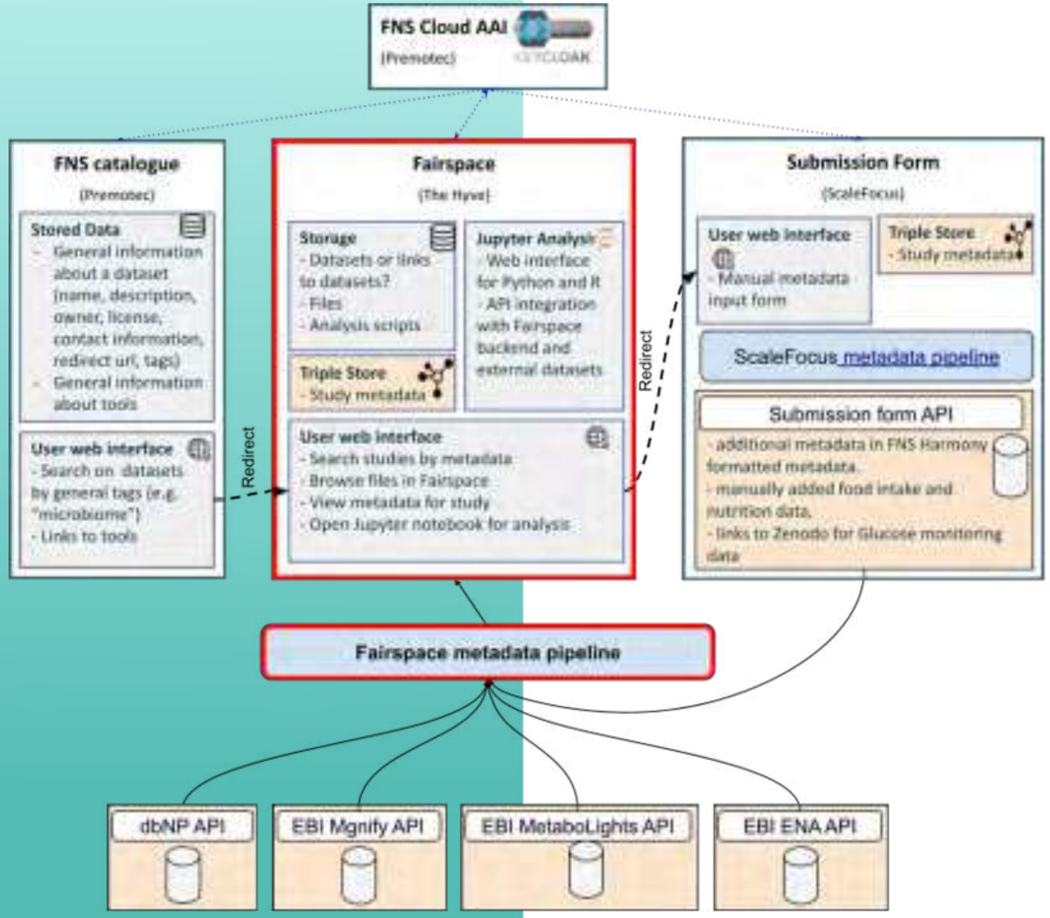
Fairspace setup for FNS-Cloud



Connection with external resources

The studies come from the following sources:

- Publicly available studies from **ENA** with a “gut microbiome” filter applied (approximately ~3500).
- Publicly available **MGnify** studies tagged with “human microbiome”.
- All publicly available **MetaboLights** studies.
- All publicly available **dbNP** studies.
- All studies submitted through the **ScaleFocus API**.

Numbers

Currently there is metadata of **over 4600 studies** uploaded to Fairspace.

For those studies are available over **653,600 samples and 3,950 subjects**.

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Customizable Metadata Model

FNS-Cloud
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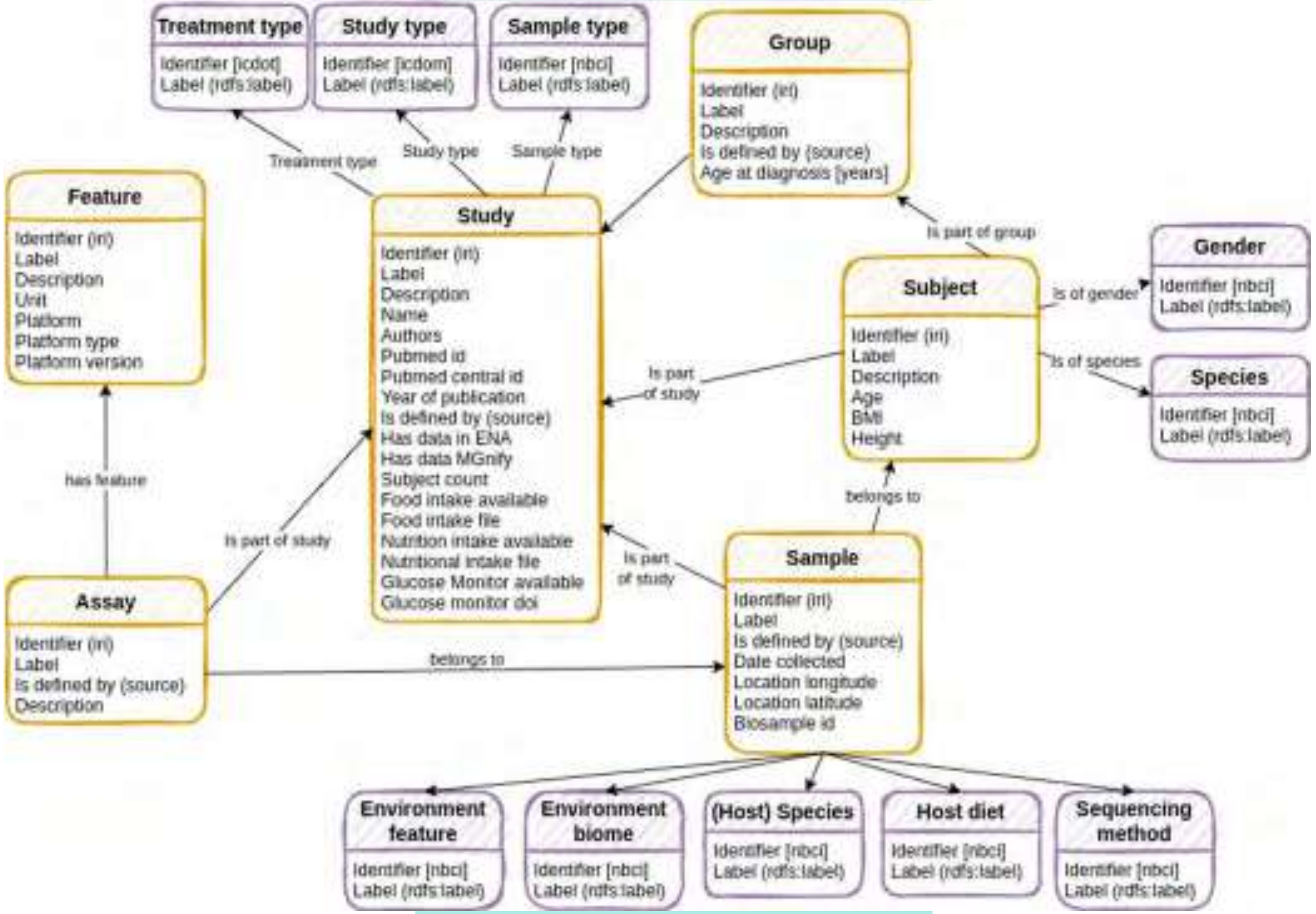
Fairspace Metadata Model

- Configurable RDF* data model, described using SHACL**
- Initial model based on dbNP, adjusted to work with ENA, MetaboLights, MGnify and others
- High level entities and properties
- Search interface adjusts automatically to the model definition



Several partners contribution (WP3): JSI, University of Florence, Maastricht University, QIB, Scalefocus

*RDF - Resource Description Framework, https://www.w3.org/RDF/
**SHACL - Shapes Constraint Language, https://www.w3.org/TR/shacl/

FNS-Cloud Food Nutrition Security

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Metadata Search & Browse Interface

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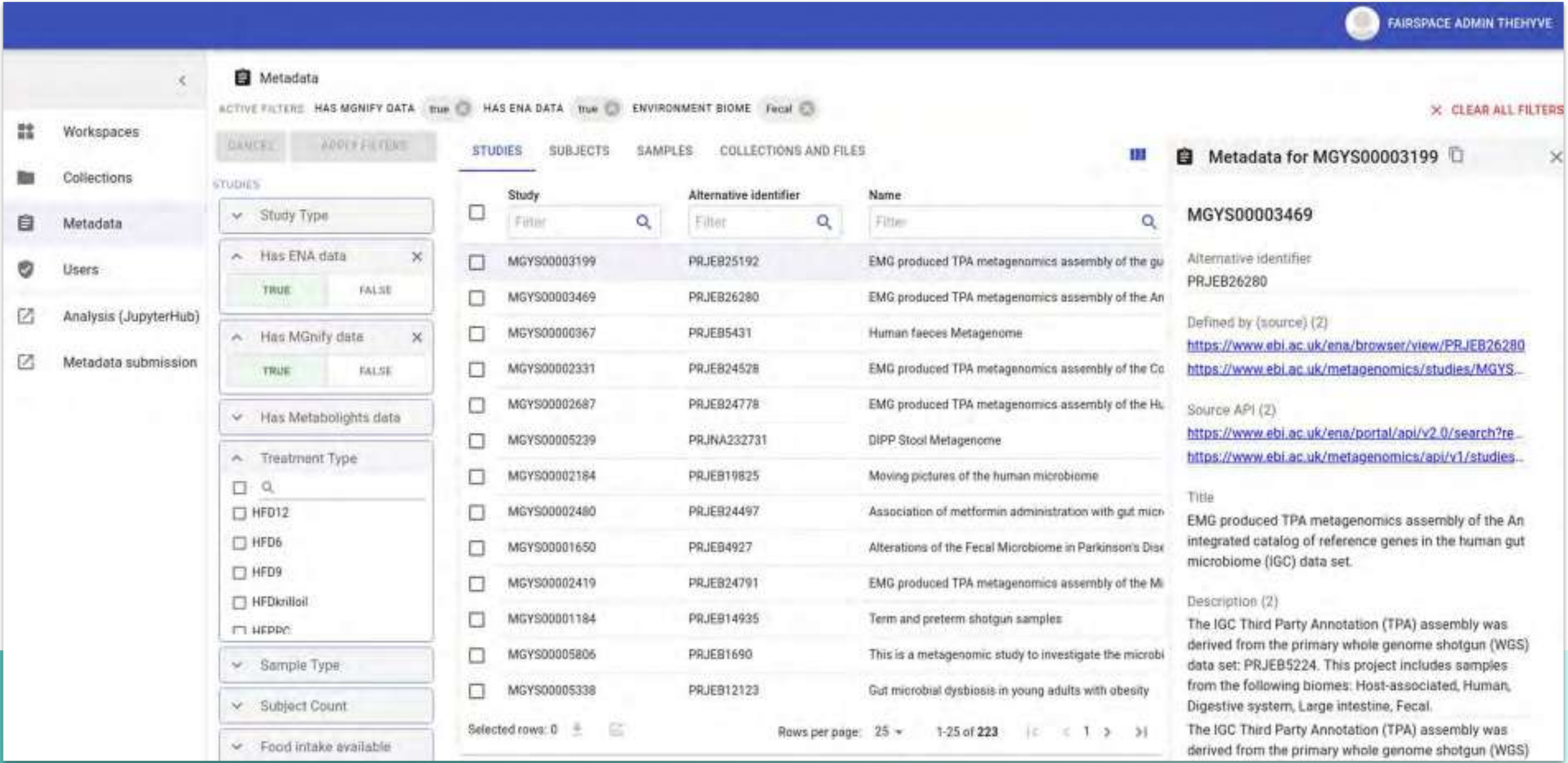

ACTIVE FILTERS HAS MGNIFY DATA true HAS ENA DATA true ENVIRONMENT BIOME Fecal

Has ENA data: TRUE FALSE

Has MGnify data: TRUE FALSE

Treatment Type
☐
☐ HFD12
☐ HFD6
☐ HFD9
☐ HFDkrilloil
☐ HFPPC

☐	Study	Alternative identifier	Name
	Filter	Filter	Filter
☐	MGYS00003199	PRJEB25192	EMG produced TPA metagenomics assembly of the gu
☐	MGYS00003469	PRJEB26280	EMG produced TPA metagenomics assembly of the An
☐	MGYS00000367	PRJEB5431	Human faeces Metagenome
☐	MGYS00002331	PRJEB24528	EMG produced TPA metagenomics assembly of the Co
☐	MGYS00002687	PRJEB24778	EMG produced TPA metagenomics assembly of the Hu
☐	MGYS00005239	PRJNA232731	DIPP Stool Metagenome
☐	MGYS00002184	PRJEB19825	Moving pictures of the human microbiome
☐	MGYS00002480	PRJEB24497	Association of metformin administration with gut micr
☐	MGYS00001650	PRJEB4927	Alterations of the Fecal Microbiome in Parkinson's Dise
☐	MGYS00002419	PRJEB24791	EMG produced TPA metagenomics assembly of the Mi
☐	MGYS00001184	PRJEB14935	Term and preterm shotgun samples
☐	MGYS00005806	PRJEB1690	This is a metagenomic study to investigate the microbi
☐	MGYS00005338	PRJEB12123	Gut microbial dysbiosis in young adults with obesity

Selected rows: 0

Rows per page: 25 1-25 of 223 1

Metadata for MGYS00003199

MGYS00003469

Alternative identifier
PRJEB26280

Defined by (source) (2)
https://www.ebi.ac.uk/ena/browser/view/PRJEB26280
https://www.ebi.ac.uk/metagenomics/studies/MGYS...

Source API (2)
https://www.ebi.ac.uk/ena/portal/api/v2.0/search?re...
https://www.ebi.ac.uk/metagenomics/api/v1/studies...

Title
EMG produced TPA metagenomics assembly of the An integrated catalog of reference genes in the human gut microbiome (IGC) data set.

Description (2)
The IGC Third Party Annotation (TPA) assembly was derived from the primary whole genome shotgun (WGS) data set: PRJEB5224. This project includes samples from the following biomes: Host-associated, Human, Digestive system, Large intestine, Fecal.
The IGC Third Party Annotation (TPA) assembly was derived from the primary whole genome shotgun (WGS)

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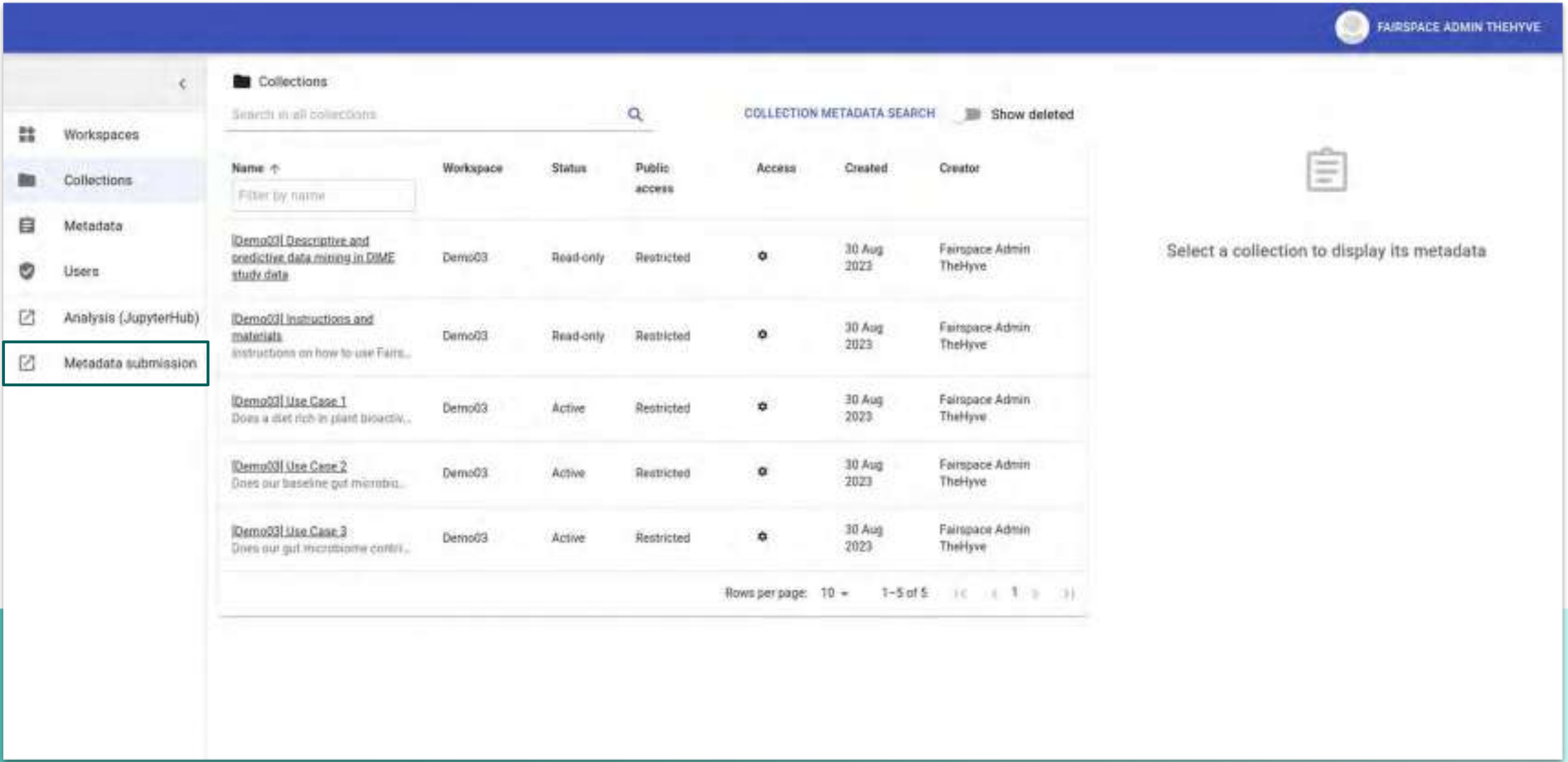
Metadata submission



Name ↑	Workspace	Status	Public access	Access	Created	Creator
[Demo03] Descriptive and predictive data mining in DIME study data	Demo03	Read-only	Restricted	⚙	30 Aug 2023	Fairspace Admin TheHyve
[Demo03] Instructions and materials Instructions on how to use Fairs...	Demo03	Read-only	Restricted	⚙	30 Aug 2023	Fairspace Admin TheHyve
[Demo03] Use Case 1 Does a diet rich in plant bioactiv...	Demo03	Active	Restricted	⚙	30 Aug 2023	Fairspace Admin TheHyve
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[Demo03] Use Case 3 Does our gut microbiome contri...	Demo03	Active	Restricted	⚙	30 Aug 2023	Fairspace Admin TheHyve

Rows per page: 10 ▾ 1–5 of 5 1

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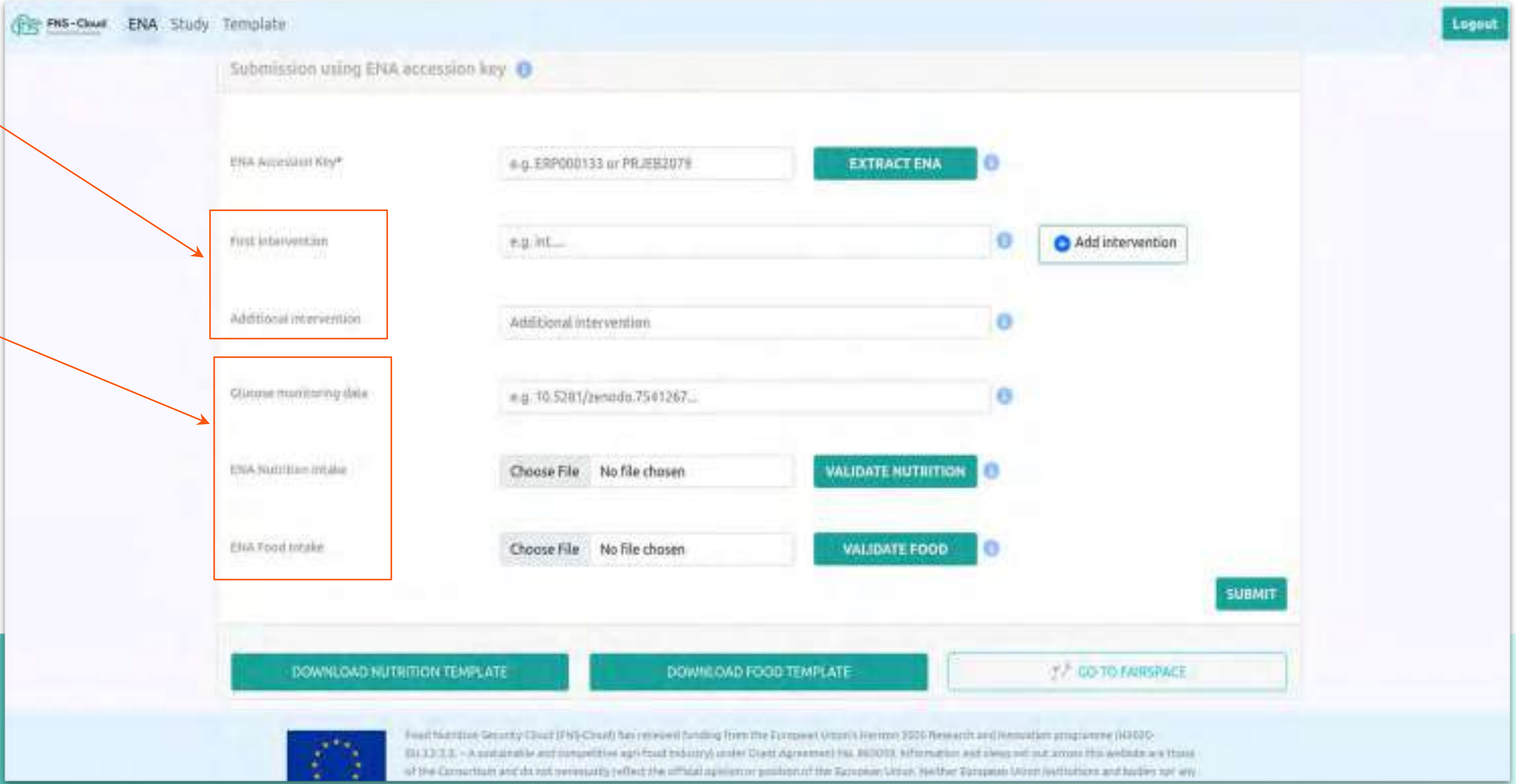
Submission form by Scalefocus

FNS-Harmony Ontology-based

Place to put data related to glucose monitoring, nutrition intake and food intake



Submission using ENA accession key

ENA Accession Key* e.g. ERP000133 or PRJEB2079

First intervention e.g. int...

Additional intervention Additional intervention

Glucose monitoring data e.g. 10.5281/zenodo.7541267...

ENA Nutrition intake No file chosen

ENA Food intake No file chosen

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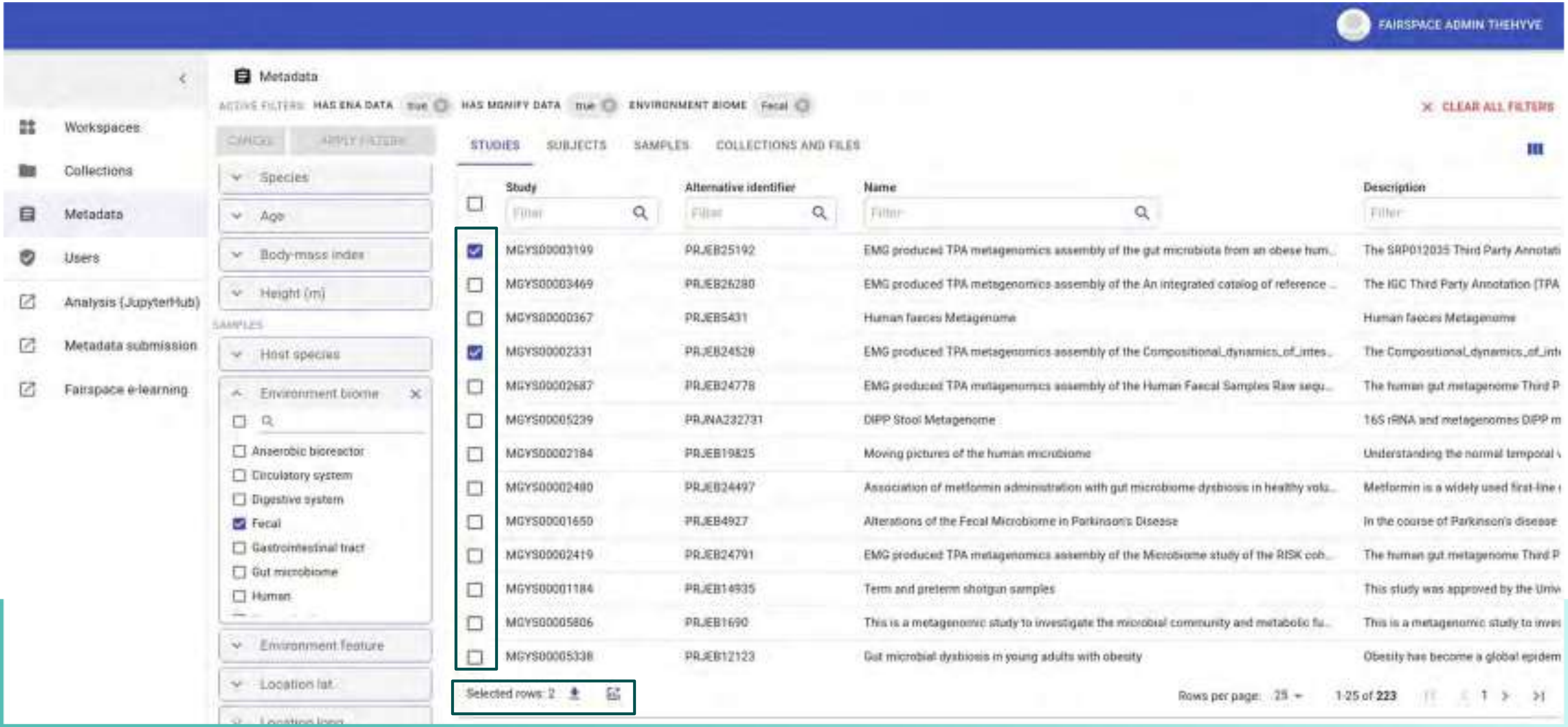
Export metadata for analysis



Metadata

ACTIVE FILTERS: HAS ENA DATA true · HAS MGNIFY DATA true · ENVIRONMENT BIOME Fecal

☐	Study	Alternative identifier	Name	Description
☑	MGYS00003199	PRJEB25192	EMG produced TPA metagenomics assembly of the gut microbiota from an obese hum...	The SRP012035 Third Party Annotati
☐	MGYS00003469	PRJEB26280	EMG produced TPA metagenomics assembly of the An integrated catalog of reference ...	The IGC Third Party Annotation (TPA
☐	MGYS00000367	PRJEB5431	Human faeces Metagenome	Human faeces Metagenome
☑	MGYS00002331	PRJEB24528	EMG produced TPA metagenomics assembly of the Compositional_dynamics_of_intes...	The Compositional_dynamics_of_inte
☐	MGYS00002687	PRJEB24778	EMG produced TPA metagenomics assembly of the Human Faecal Samples Raw sequ...	The human gut metagenome Third P
☐	MGYS00005239	PRJNA232731	DIPP Stool Metagenome	16S rRNA and metagenomes DIPP m
☐	MGYS00002184	PRJEB19825	Moving pictures of the human microbiome	Understanding the normal temporal v
☐	MGYS00002480	PRJEB24497	Association of metformin administration with gut microbiome dysbiosis in healthy volu...	Metformin is a widely used first-line (
☐	MGYS00001650	PRJEB4927	Alterations of the Fecal Microbiome in Parkinson's Disease	In the course of Parkinson's disease
☐	MGYS00002419	PRJEB24791	EMG produced TPA metagenomics assembly of the Microbiome study of the RISK coh...	The human gut metagenome Third P
☐	MGYS00001184	PRJEB14935	Term and preterm shotgun samples	This study was approved by the Univ
☐	MGYS00005806	PRJEB1690	This is a metagenomic study to investigate the microbial community and metabolic fu...	This is a metagenomic study to inves
☐	MGYS00005338	PRJEB12123	Gut microbial dysbiosis in young adults with obesity	Obesity has become a global epidem

Selected rows: 2

Rows per page: 25 · 1-25 of 223 · 1

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Integrated Analysis Environment

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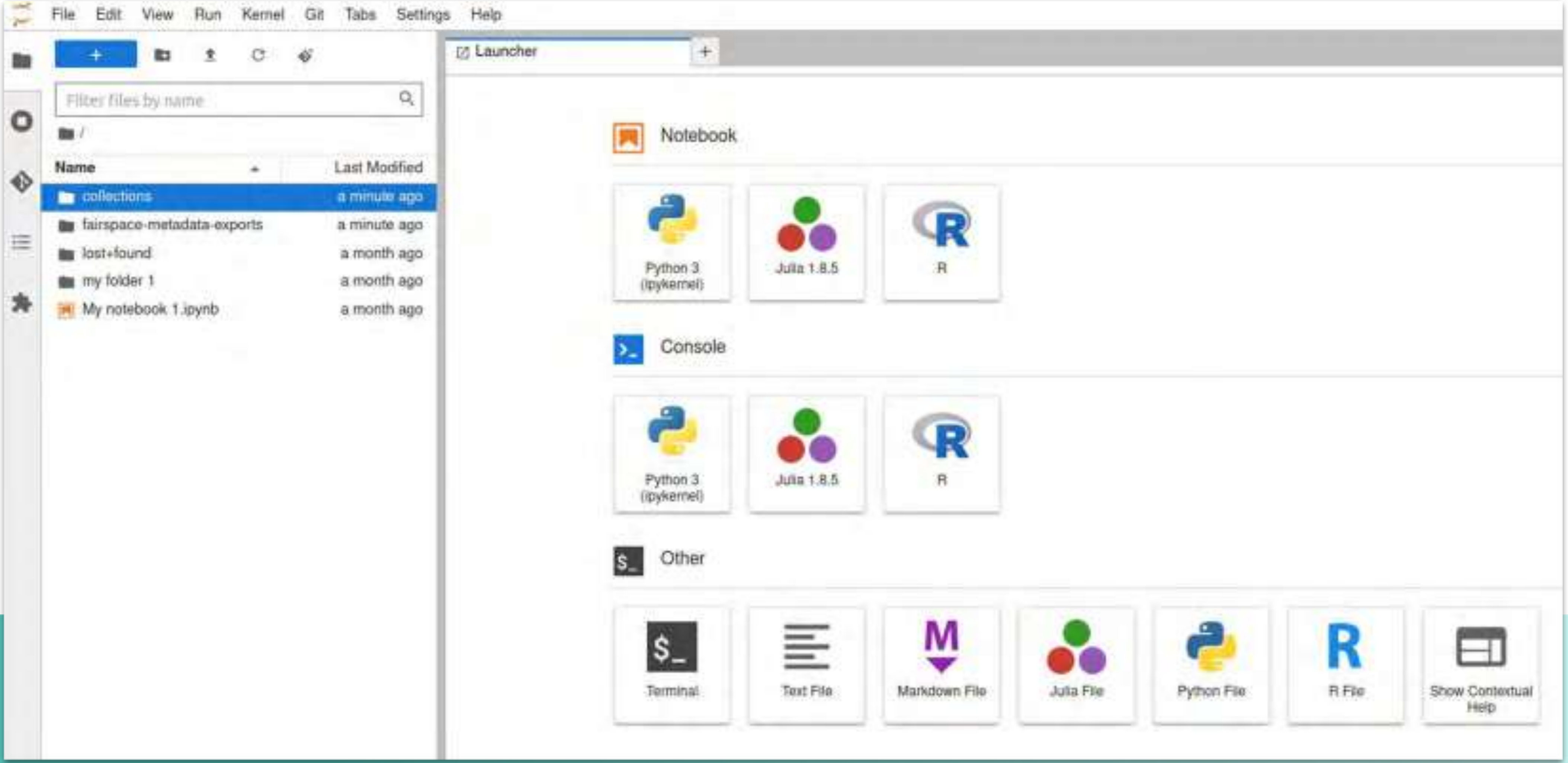
Analysis - integrated Jupyter environment



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Secure File storage Collections

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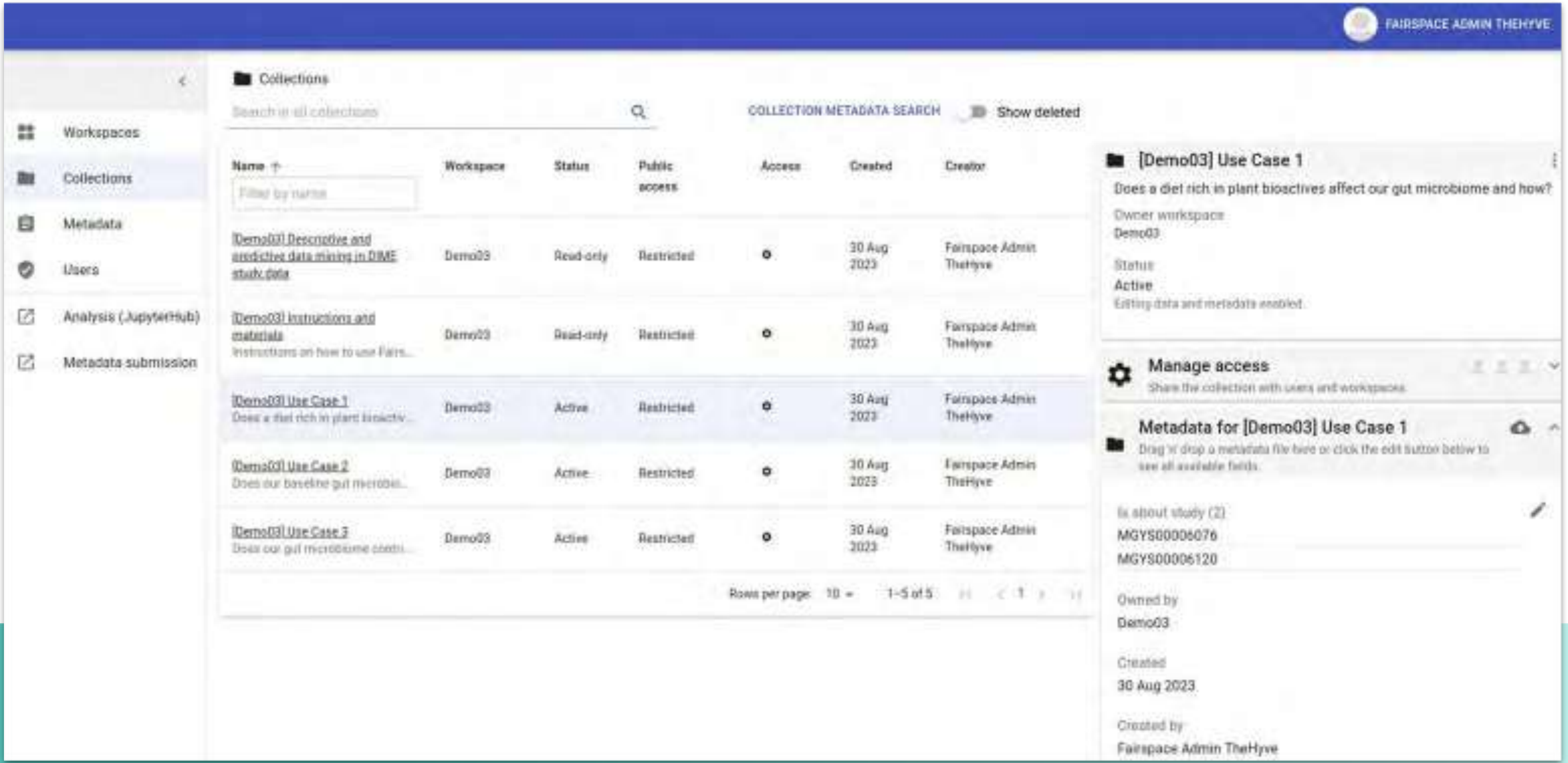
Fairspace Collections



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[Demo03] Use Case 3 Does our gut microbiome contri...	Demo03	Active	Restricted	●	30 Aug 2023	Fairspace Admin TheHyve

[Demo03] Use Case 1

Does a diet rich in plant bioactives affect our gut microbiome and how?

Owner workspace
Demo03

Status
Active
Editing data and metadata enabled

Manage access
Share the collection with users and workspaces

Metadata for [Demo03] Use Case 1
Drag 'n' drop a metadata file here or click the edit button below to see all available fields

Is about study (2)
MGYS00006076
MGYS00006120

Owned by
Demo03

Created
30 Aug 2023

Created by
Fairspace Admin TheHyve

QIB scripts

Usecase 1,2,3

UM scripts

Usecase 1

JSI scripts

Descriptive and predictive data mining

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Fairspace Workspaces

Demo03

Title
Demonstrative workspace with shared analysis scripts

Workspace description

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Workspace contains scripts for three research questions demonstrating how FNS-Cloud and Fairspace facilitates analyses of microbiomes that improves our understanding of the interaction between diet and microbiome.

It also contains additional descriptive and predictive data mining in DIME study data, as well as instructions and other materials for the users.

Keywords (4)
analysis scripts
demonstrator
FNS-Cloud
microbiome

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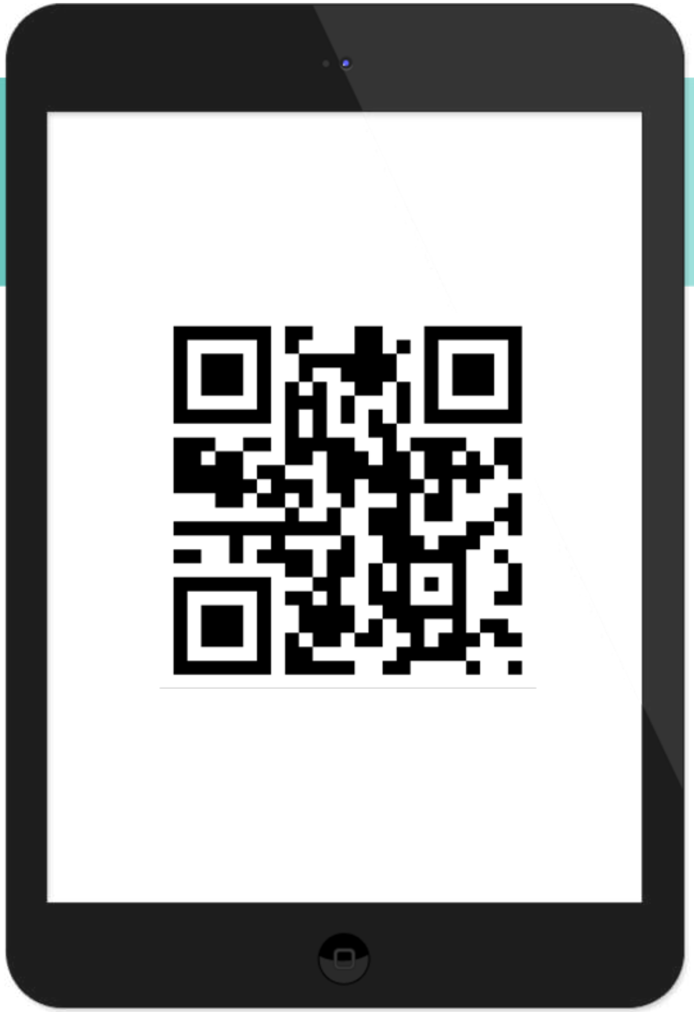
Login into Fairspace



- Register to FNS-Cloud if you do not have the credentials yet
- Start Analysis JupyterHub

https://demo.fns-fairspace.app

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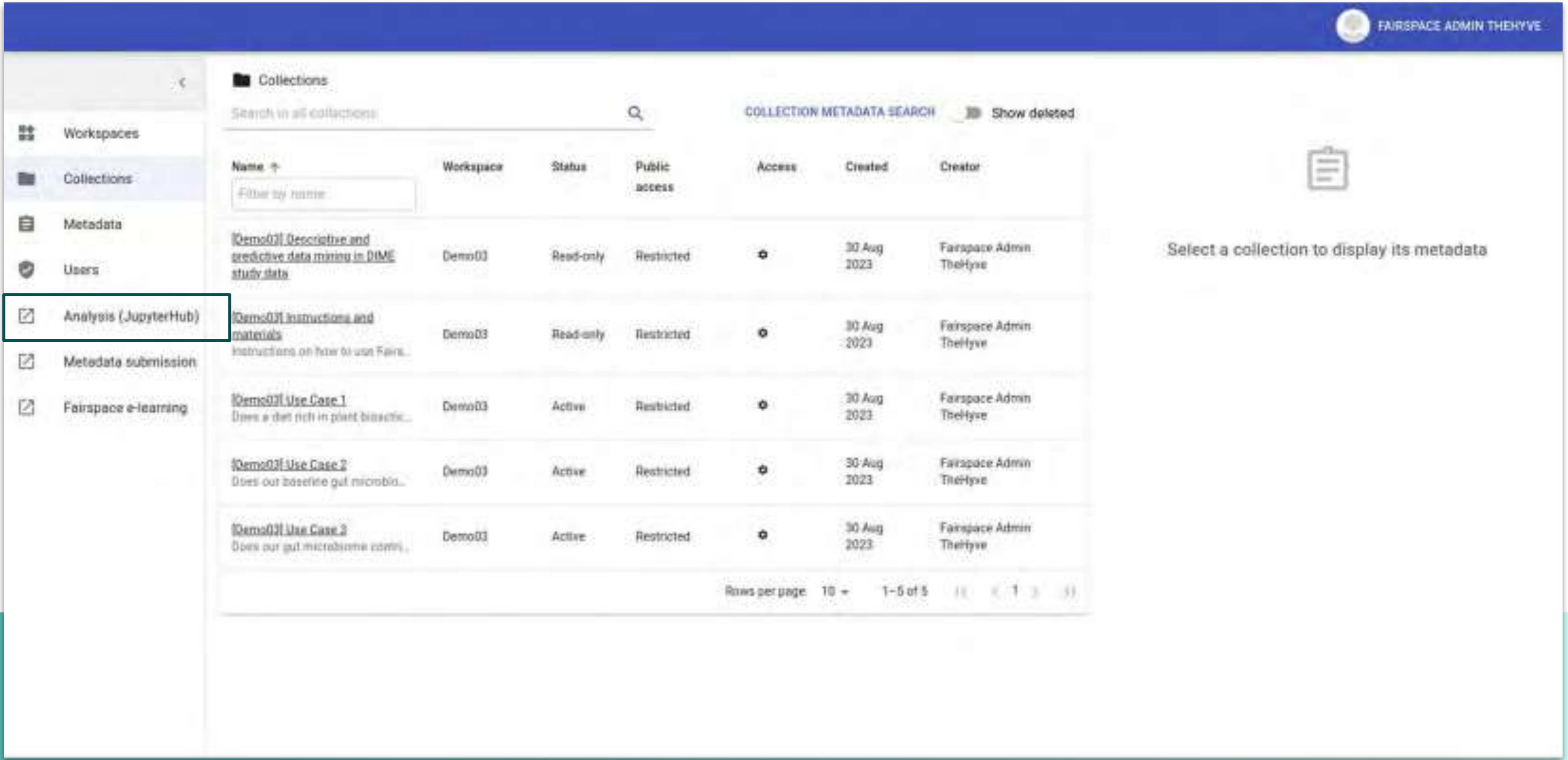
Open Analysis (JupyterHub) Tab and Start Jupyter



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Rows per page 10 ▾ 1–5 of 5 |‹ ‹ 1 › ›|

Select a collection to display its metadata

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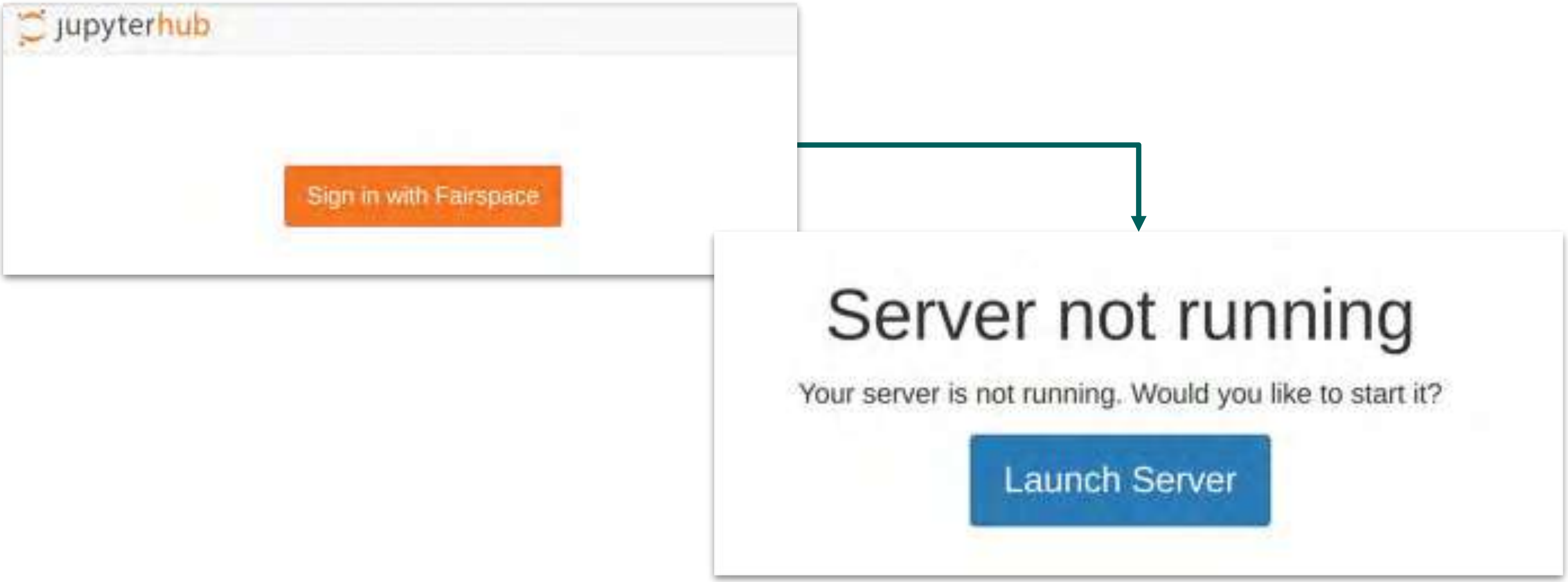
Starting JupyterHub



Server not running

Your server is not running. Would you like to start it?

FNS - Cloud
Food Nutrition Security

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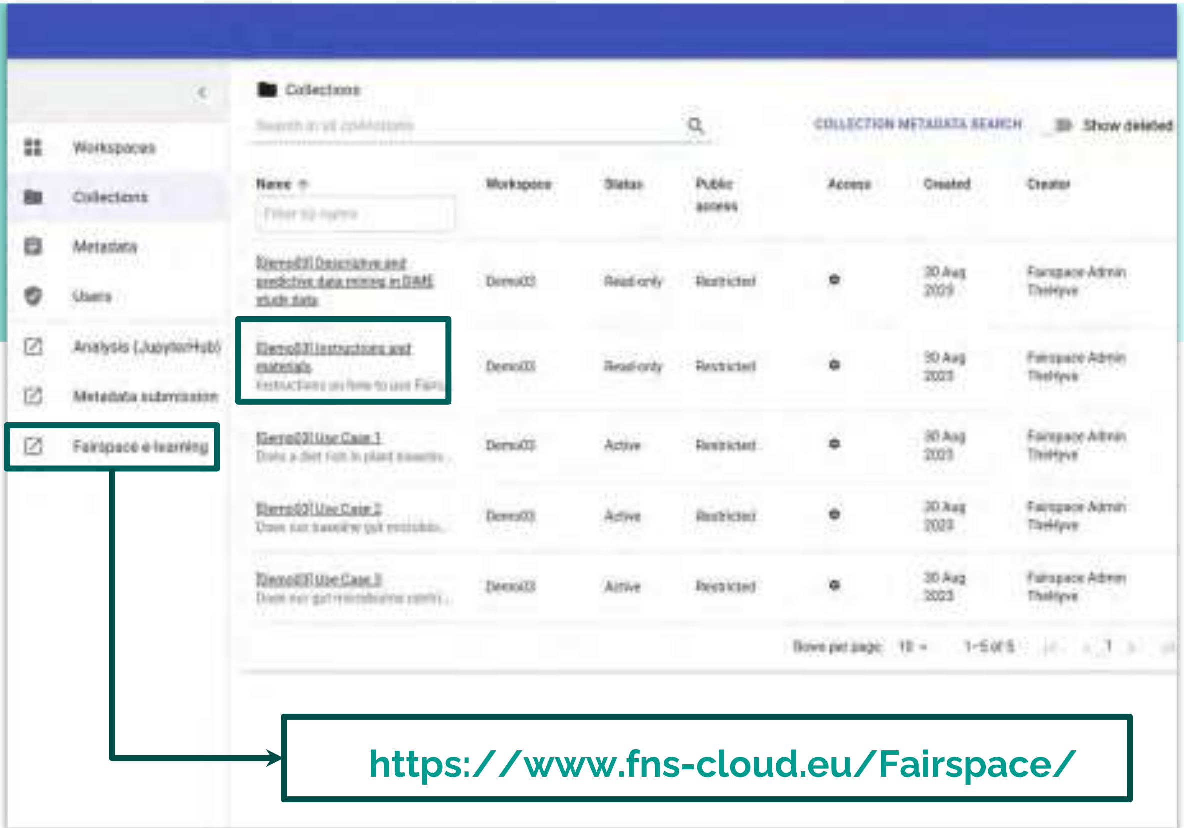
Fairspace
Hands on session

https://demo.fns-fairspace.app



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[Demo03] Use Case 3	Demo03	Active	Restricted	●	30 Aug 2023	Fairspace Admin TheHyve

Rows per page: 10 1–5 of 5

https://www.fns-cloud.eu/Fairspace/

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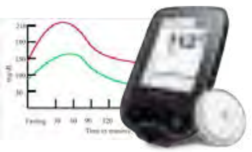
Demonstrator Use Cases

RESEARCH Q1: Does a diet rich in plant bioactives affect our gut microbiome, and how?

- demonstrate user pathway
- the metagenomics and metabolomics datasets and bioinformatic analytical pipelines (handling emerging metagenomics datasets for higher resolution microbial analysis e.g. long-read sequencing)

RESEARCH Q2: Does our baseline gut microbiome define how species composition shifts upon dietary interventions?

- Finding, accessing and merging datasets from different diet & microbiome studies



RESEARCH Q3: Does our gut microbiome contribute to our metabolic response to foods? Can we predict metabolic responses to foods using microbiome data? Is there more to food than nutrients?

- How a user can access multiple datasets and a new **WP3** machine-learning prediction tool

FNS-Cloud
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Let us know what you think

- **further development**
  - What do you want to see in next generation Fairspace?
- **engaging user communities**
  - Would you use this in your work?
  - How can we promote this better?

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Don't forget to follow us: @FNSCloudEU FNSCloudEU FNS-Cloud @FNSCloudEU2019

www.fns-cloud.eu
www.fnscloud.eu
www.myfnscloud.eu

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